CO Coupling Chemistry of a Terminal Mo Carbide: Sequential Addition of Proton, Hydride, and CO Releases Ethenone

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Supporting Information

Contents

EXPERIMENTAL DETAILS

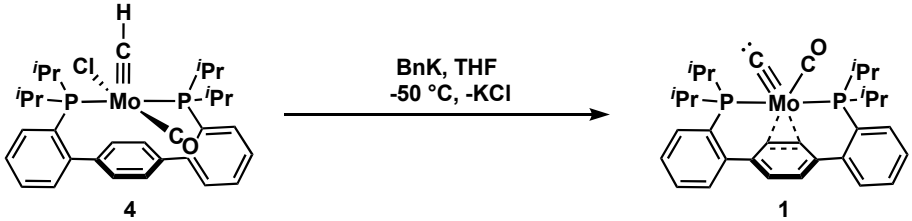
General Considerations

Note. *Below, we distinguish the ^{13}C-labelled compounds from their non-labelled derivatives by adding the modifier "**-^{13}C**" after the compound number. In the main article, this modifier is omitted for clarity, as mainly the ^{13}C-labelled compounds are discussed.*

Unless otherwise specified, all operations were carried out in an MBraun drybox under a nitrogen atmosphere or using standard Schlenk and high vacuum line techniques. Solvents for air- and moisture-sensitive reactions were dried over sodium benzophenone ketyl, or by the method of Grubbs.[1] C_6D_6 was purchased from Cambridge Isotope Laboratories and vacuum transferred from sodium benzophenone ketyl. Solvents, once dried and degassed, were vacuum transferred directly prior to use or stored under inert atmosphere over 4 Å molecular sieves. Molybdenum complexes **9**[2] and **12**;[3] trimethylsilyl ketene;[4] anhydrous tetrabutylammonium fluoride (TBAF) in MeCN;[5] benzyl potassium;[6] and $PhAr_2PMeCl$ (Ar = 2,4,6-trimethoxyphenyl)[7] were prepared and purified according to literature procedures. $[Et_3NH][Cl]$ was prepared by condensing HCl gas (freeze-pump-thawed three times and condensed from -78 to -196 °C) onto a frozen pentane solution of dry NEt_3. The solids that formed upon warming to room temperature (with stirring) were collected via vacuum filtration and used without further purification. P2Et•HCl was prepared by addition of 1.0 M HCl in anhydrous Et_2O (1.1 equiv) to P2Et in THF, followed by concentrating in vacuo to dryness. NaH (purchased as 60% dispersion in mineral oil; Sigma Aldrich) was purified by rinsing with copious pentane and then drying in vacuo. All other chemicals were utilized as received. Trimethylsilyl chloride (dried over CaH_2 and distilled prior to use) was purchased from Alfa Aesar. Sodium triethylborohydride ($NaBEt_3H$, 1.0 M in PhMe), triphenylborane, sodium tetraphenylborate, phosphazene base P2Et, anhydrous HCl (1.0 M solution in Et_2O), HCl (gas, ≥99%) ,and CO (≥99%) were purchased from Sigma Aldrich. NEt_3 (dried over CaH_2 and distilled prior to use) was purchased from Oakwood Chemicals. ^{13}CO gas was purchased from Monsanto Research; and butane was purchased from Matheson. ^{1}H, ^{13}C{^{1}H}, and ^{31}P{^{1}H} NMR spectra were recorded on Varian 300 MHz, 400 MHz, Varian INOVA-500, or Varian 600 MHz spectrometers with chemical shifts reported in parts per million (ppm). ^{1}H and ^{13}C{^{1}H} NMR spectra are referenced to residual solvent peaks.[8] ^{31}P{^{1}H} chemical shifts are referenced to an external sample of 85% H_3PO_4 (0 ppm). Multiplicities are abbreviated as follows: s = singlet, d = doublet, t = triplet, dd = doublet of doublets, dt = doublet of triplets, td = triplet of doublets, m = multiplet, br = broad, and app = apparent. Infrared (IR) spectra were collected on a Bruker Alpha II FTIR spectrometer equipped with an ATR sampling accessory. Elemental analysis was performed using a PerkinElmer 2400 Series II CHN Elemental Analyzer.

Carbide–CO Coupling from Carbide 1

*In Situ Generation of Carbide **1***



4 **1**

For synthesis of methylidyne **4**, see below. A J. Young NMR tube was charged with solid **4** (25 mg. 0.039 mmol) and solid BnK (5.1 mg, 0.039 mmol). The tube was sealed and appended to a high vacuum manifold. The tube was thoroughly evacuated and THF (*ca.* 0.5 mL) was admitted via vacuum transfer by cooling the reaction tube to -78 °C with a dry ice/acetone slurry. The tube was sealed and carefully mixed, ensuring that the reaction solution remained cold. The orange solids dissolved, providing a deep red homogeneous solution.

The J. Young tube was carefully transferred to an NMR probe pre-cooled to -50 °C. Multinuclear NMR spectroscopy showed complete conversion of **4** to previously characterized carbide complex **1** (Fig. S1).[2]

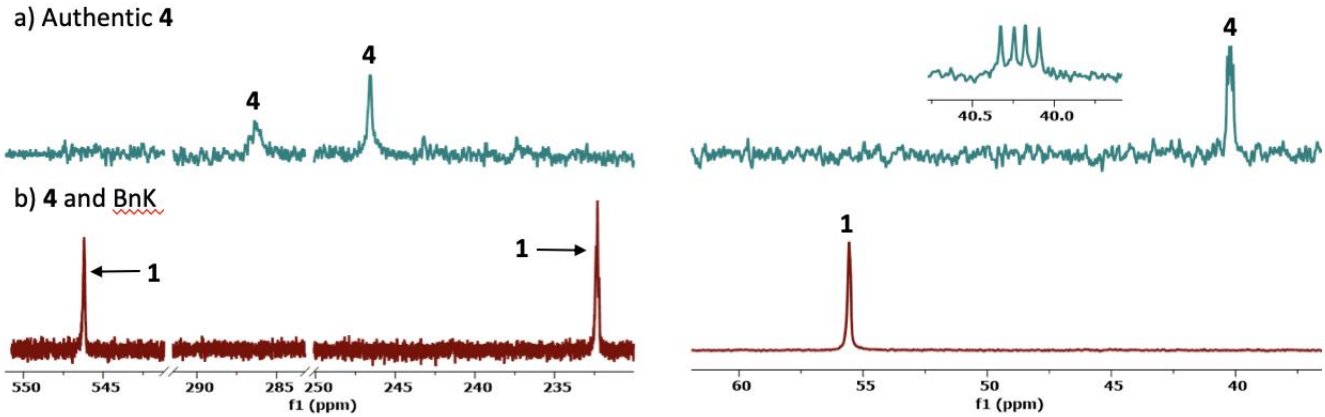
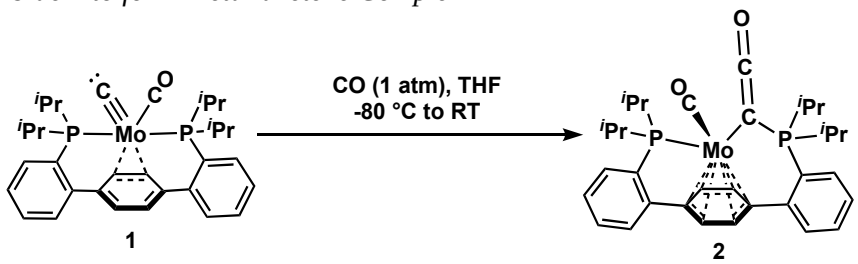


Figure S1—Partial $^{13}C\{^{1}H\}$ (126 MHz, THF, -50 °C; left) and $^{31}P\{^{1}H\}$ (202 MHz, THF, -50 °C; right) NMR spectra demonstrating the clean deprotonation of methylidyne **4** with benzyl potassium.

*Addition of CO to Carbide **1** to form Metallaketene Complex **2***



A deep red THF solution of **1** (0.047 mmol in 600 μL THF) in a J. Young tube, prepared as above, was degassed via three freeze pump thaw cycles (thawing to -78 °C). The headspace was backfilled with CO gas (1 atm) at -78 °C, and then warmed to RT, resulting in a darkening of the reaction mixture to brown. After 2 h at RT, volatiles were removed in vacuo. The resulting brown residue was triturated with hexanes (3x5 mL), and then washed with hexamethyldisiloxane (HMDSO; 5x5 mL). The remaining solids was extracted with benzene (5 mL), and the benzene extracts lyophilized to provide **2** as a red-brown, free-flowing solid (5 mg, 17%). ^{1}H NMR (C_6D_6, 400 MHz, 23 °C): 7.60 – 7.52 (overlapping m, 2H, aryl-*H*), 7.36 – 7.29 (m, 1H, aryl-*H*), 7.12 – 6.99 (m, 3H, aryl-*H*), 6.86 – 6.80 (m, 1H, aryl-*H*), 6.75 – 6.67 (m, 1H, aryl-*H*), 4.84 – 4.77 (m, 2H, central arene-*H*), 3.98 – 3.89 (m, 2H, central arene-*H*), 3.15 – 3.00 (m, 1H, C*H*$(CH_3)_2$), 2.83 – 2.68 (m, 1H, C*H*$(CH_3)_2$), 2.01 – 1.87 (m, 1H, C*H*$(CH_3)_2$), 1.88 – 1.73 (m, 1H, C*H*$(CH_3)_2$), 1.68 (dd, J = 15.9 Hz, J = 6.9 Hz, 3H, CH(C*H*$_3)_2$), 1.50 – 1.36 (m, 6H, CH(C*H*$_3)_2$), 1.14 – 0.99 (m, 6H, CH(C*H*$_3)_2$), 0.92 – 0.73 (m, 12H, CH(C*H*$_3)_2$). $^{13}C\{^{1}H\}$ NMR (C_6D_6, 126 MHz, 23 °C): 242.90 (d, $^{2}J_{PC}$ = 13.1 Hz, *C*O), 150.64 (d, J = 26.8 Hz, aryl-*C*), 149.78 (d, $^{2}J_{PC}$ = 1.7 Hz, aryl-*C*), 150.02 (d, $^{2}J_{PC}$ = 33.3 Hz, PC*C*O), 148.63 (d, $^{2}J_{PC}$ = 29.4 Hz, aryl-*C*), 132.54 (d, $^{2}J_{PC}$ = 6.0 Hz, aryl-*C*), 131.70 (d, $^{2}J_{PC}$ = 11.7 Hz, aryl-*C*), 126.82 (d, $^{2}J_{PC}$ = 4.2 Hz, aryl-*C*), 124.64 (d, $^{2}J_{PC}$ = 12.4 Hz, aryl-*C*), 99.93 (s, central arene-*C*), 95.60 (s, central arene-*C*), 87.41 (s, central arene-*C*), 77.73 (dd, J = 7.6 Hz, J = 5.4 Hz, central arene-*C*), 74.51 (s, central arene-*C*), 73.62 (s, central arene-*C*), 30.84 (d, J = 49.8 Hz, *C*H$(CH_3)_2$), 29.34 (d, J = 52.4 Hz, *C*H$(CH_3)_2$), 27.42 (d, J = 20.4 Hz, *C*H$(CH_3)_2$), 24.50 (d, J = 10.0 Hz, *C*H$(CH_3)_2$), 21.91 (d, J = 9.5 Hz, CH(*C*H$_3)_2$), 18.82 (d, J = 5.6 Hz, CH(*C*H$_3)_2$), 18.14 (d, J = 5.1 Hz, CH(*C*H$_3)_2$), 17.77 (d, J = 8.0 Hz, CH(*C*H$_3)_2$), 17.52 (d, J = 1.8 Hz, CH(*C*H$_3)_2$), 17.08 (d, J = 2.1 Hz, CH(*C*H$_3)_2$), 16.57 (d, J = 1.1 Hz, CH(*C*H$_3)_2$), 16.24 (d, J = 1.1 Hz, CH(*C*H$_3)_2$), -32.00 (d, $^{1}J_{PC}$ = 119 Hz, P*C*CO). $^{31}P\{^{1}H\}$ NMR (C_6D_6, 202 MHz, 23 °C): 83.45 (d, $^{2}J_{PP}$ = 4.5 Hz, *P*Mo), 38.29 (d, $^{3}J_{PP}$ = 4.4 Hz, *P*CCO). FTIR (ATR, cm^{-1}): 2029 (s, C=C=O), 1802 (s, C≡O).

2-^{13}C can be prepared analogously, starting from **1-^{13}C** and ^{13}CO. Key data: ^{31}P{^{1}H} NMR (THF, 202 MHz, 23 °C): 81.69 (dd, $^{2}J_{PC}$ = 12.6 Hz, & $^{3}J_{PP}$ = 4.1 Hz, *P*Mo), 37.64 (ddd, $^{1}J_{PC}$ = 118.1 Hz, $^{2}J_{PC}$ = 33.2 Hz, & $^{3}J_{PP}$ = 4.2 Hz, *P*CCO). ^{13}C{^{1}H} NMR (THF, 126 MHz, 23 °C): 241.64 (d, $^{2}J_{PC}$ = 13.0 Hz, *C*O), 149.54 (dd, $^{1}J_{CC}$ = 103 Hz, $^{2}J_{PC}$ = 33.2 Hz, PC*C*O), -32.14 (dd, $^{1}J_{PC}$ = 118 Hz, $^{1}J_{CC}$ = 103 Hz, P*C*CO).

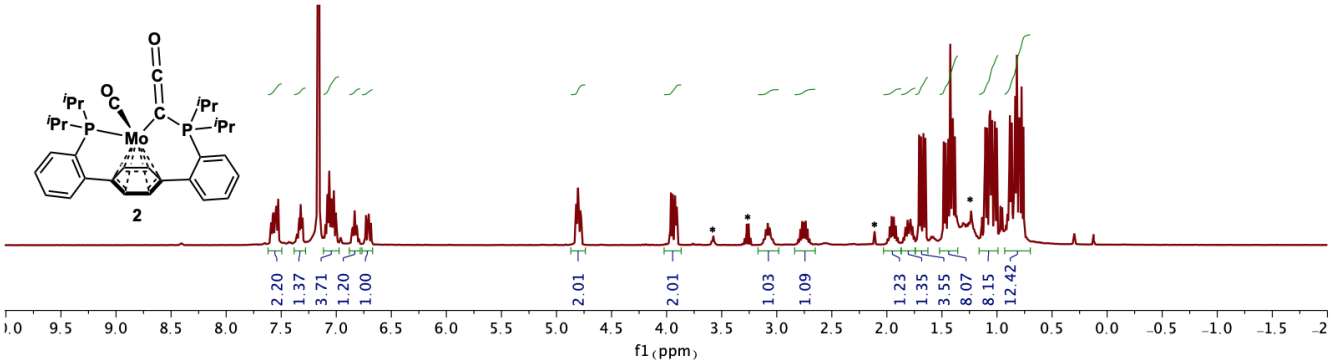


Figure S2—^{1}H NMR Spectrum (400 MHz, C_6D_6, 23 °C) of **2**. (*) denotes residual solvents (Et_2O, THF, hexanes, toluene).

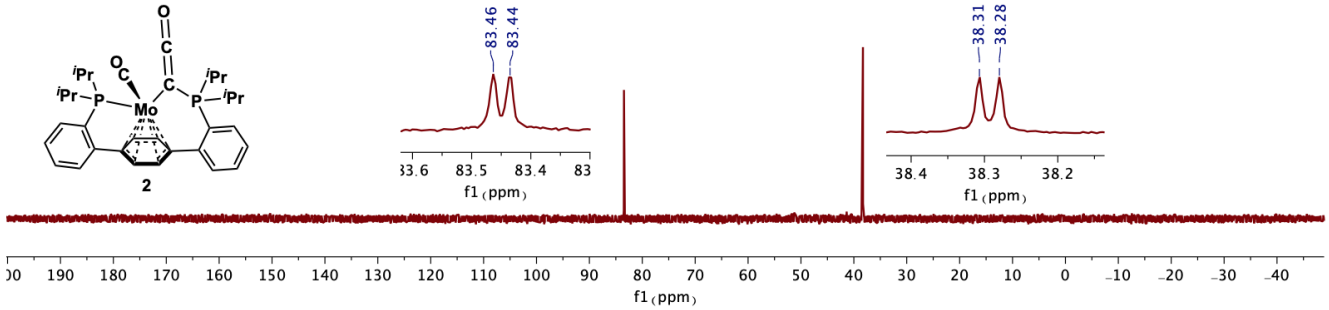


Figure S3—^{31}P{^{1}H} NMR Spectrum (162 MHz, C_6D_6, 23 °C) of **2**.

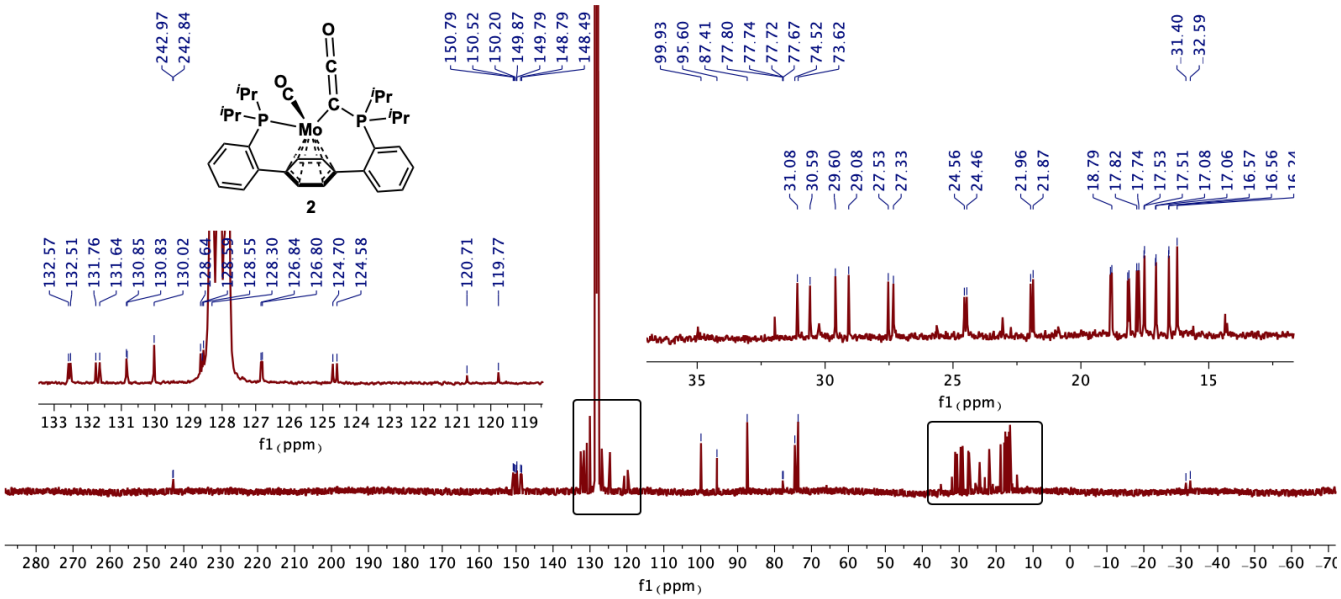


Figure S4—$^{13}C\{^{1}H\}$ NMR Spectrum (101 MHz, C_6D_6, 23 °C) of **2**. The insets magnify crowded regions of the spectrum.

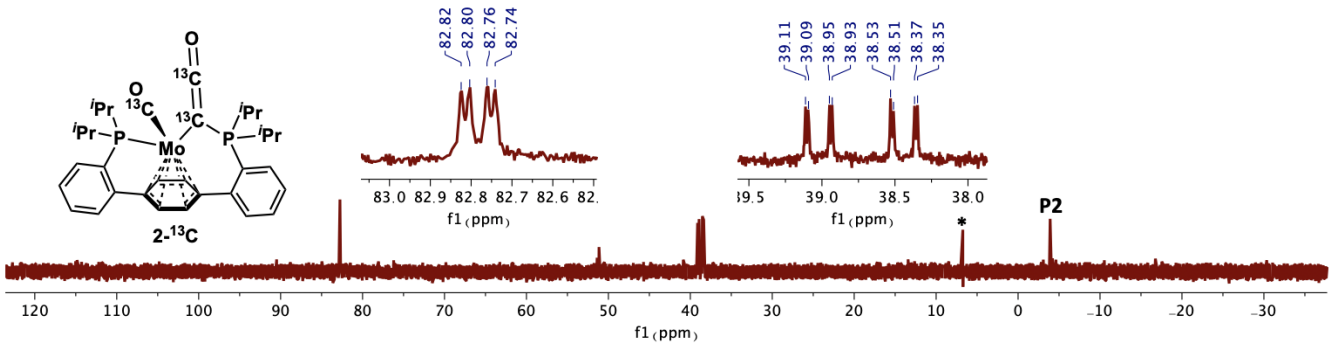


Figure S5—$^{31}P\{^{1}H\}$ NMR spectrum (202 MHz, THF, 23 °C) of **2-^{13}C**. (*) Denotes a data artifact. A small amount of free P2 ligand (indicative of decomposition) is denoted at –3.91 ppm.

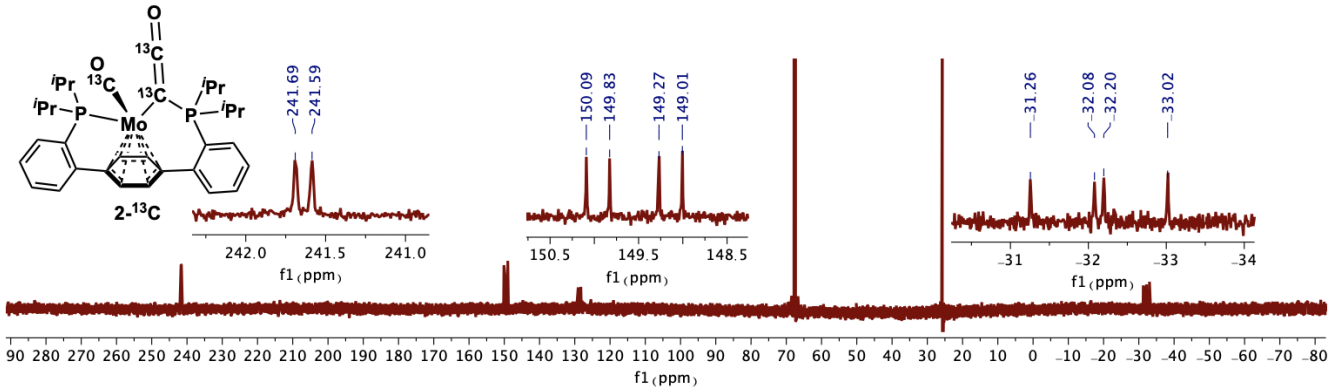
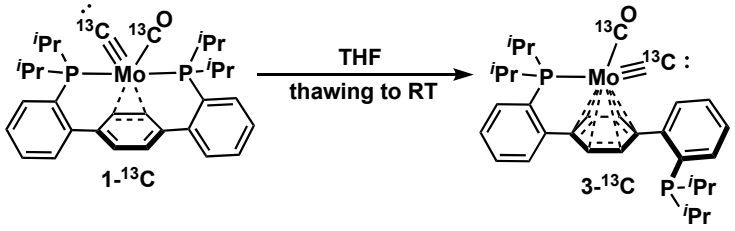


Figure S6—$^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, THF, 23 °C) of **2-^{13}C**. The insets magnify the ^{13}C-enriched signals.

*Preparation of a mixture predominantly comprised of carbide isomer **3-^{13}C***



3-^{13}C is observed as the primary product on warming solutions of **1-^{13}C**, generated *in situ* via deprotonation of **4-^{13}C** (see above), to RT over several hours. However, purification was not attempted from these reactions. The spectra presented in Figures S7-S9 were collected from a sample generated as follows:

A THF solution of **1-^{13}C** was prepared via an adaptation of the reported procedure[2]: a 20 mL scintillation vial was charged with **9-^{13}C** (50 mg, 0.070 mmol), THF (*ca*. 2 mL), and a stir bar. The contents of the vial were frozen solid in an LN_2-chilled cold well. Anhydrous tetrabutylammonium fluoride (18.3 mg, 0.070 mmol) was added as a solid and the solution allowed to thaw with stirring. Moving the vial in and out of the cold well, the reaction was stirred while maintaining a temperature of 0 to -20 °C (as determined by an external low-temperature alcohol thermometer pressed against the side of the vial) for approximately 30 mins, to promote formation of **1-^{13}C**.

The resulting red solution was placed in a -35 °C freezer for 12 h. At this time, the reaction solution had darkened significantly. Volatiles were removed under reduced pressure, affording a dark residue (NB: during this time, no special precautions were taken to prevent sample warming). After thorough trituration of the resulting solids with hexanes (4 mL x 3), HMDSO (5 mL) was added and the suspension filtered through a Celite plug. The filter cake was extracted with HMDSO until the washes were colorless. The resulting deep purple filtrate solution was concentrated *in vacuo* until solids began to form. After standing at -35 °C for 48 h, the mixture was rapidly filtered through pre-cooled 2 mL medium porosity fritted funnel, affording a dark purple solid. The solid was washed into a clean 20 mL scintillation vial with benzene (*ca.* 2 mL), the solution lyophilized, C_6D_6 (500 μL) added, and the resulting solution characterized immediately by multinuclear NMR spectroscopy. The predominant species can be assigned as **3-^{13}C**, though impurities are present. The reaction yield was not determined. ^{1}H NMR (C_6D_6, 400 MHz, 23 °C): 8.11-8.14 (m, 1H, aryl-*H*), 7.18 (d, *J* = 7.7 Hz, 1H, aryl-*H*), 6.99 (t, *J* = 5.2 Hz, 2H, aryl-*H*), 6.96 – 6.87 (m, 3H, aryl-*H*), 6.79 (td, *J* = 7.4, 1.4 Hz, 1H, aryl-*H*), 6.27 (d, *J* = 6.3 Hz, 1H, central arene-*H*), 4.61 (d, *J* = 6.1 Hz, 1H, central arene-*H*), 4.54 (d, *J* = 6.3 Hz, 1H, central arene-*H*), 3.38 (d, *J* = 6.4 Hz, 1H, central arene-*H*), 2.49 – 2.60 (m, 1H, C*H*(CH_3)$_2$), 2.09 – 2.21 (m, 1H, C*H*(CH_3)$_2$), 1.86 – 1.94 (m, 1H, C*H*(CH_3)$_2$), 1.67 – 1.74 (m, 1H, C*H*(CH_3)$_2$), 1.52 (dd, *J* = 17.0, 6.8 Hz, 3H, CH(C*H*$_3$)$_2$), 1.27 (dd, *J* = 12.1, 6.9 Hz, 3H, CH(C*H*$_3$)$_2$), 1.10 (dd, *J* = 14.5, 6.9 Hz, 3H, CH(C*H*$_3$)$_2$), 1.04 – 0.95 (m, 3H, CH(C*H*$_3$)$_2$), 0.91 (dd, *J* = 12.5, 7.0 Hz, 3H, CH(C*H*$_3$)$_2$), 0.82 (dd, *J* = 14.5, 7.0 Hz, 3H, CH(C*H*$_3$)$_2$), 0.70 (dd, *J* = 15.6, 6.8 Hz, 3H, CH(C*H*$_3$)$_2$), 0.53 (dd, *J* = 10.4, 6.9 Hz, 3H, CH(C*H*$_3$)$_2$). ^{13}C{^{1}H} NMR (C_6D_6, 101 MHz, 23 °C): 569.92 (br s, Mo≡*C*:), 213.03 (s, Mo-*C*O). ^{31}P{^{1}H} NMR (C_6D_6, 162 MHz, 23 °C): 91.48 (s, *P*Mo), -4.08 (s).

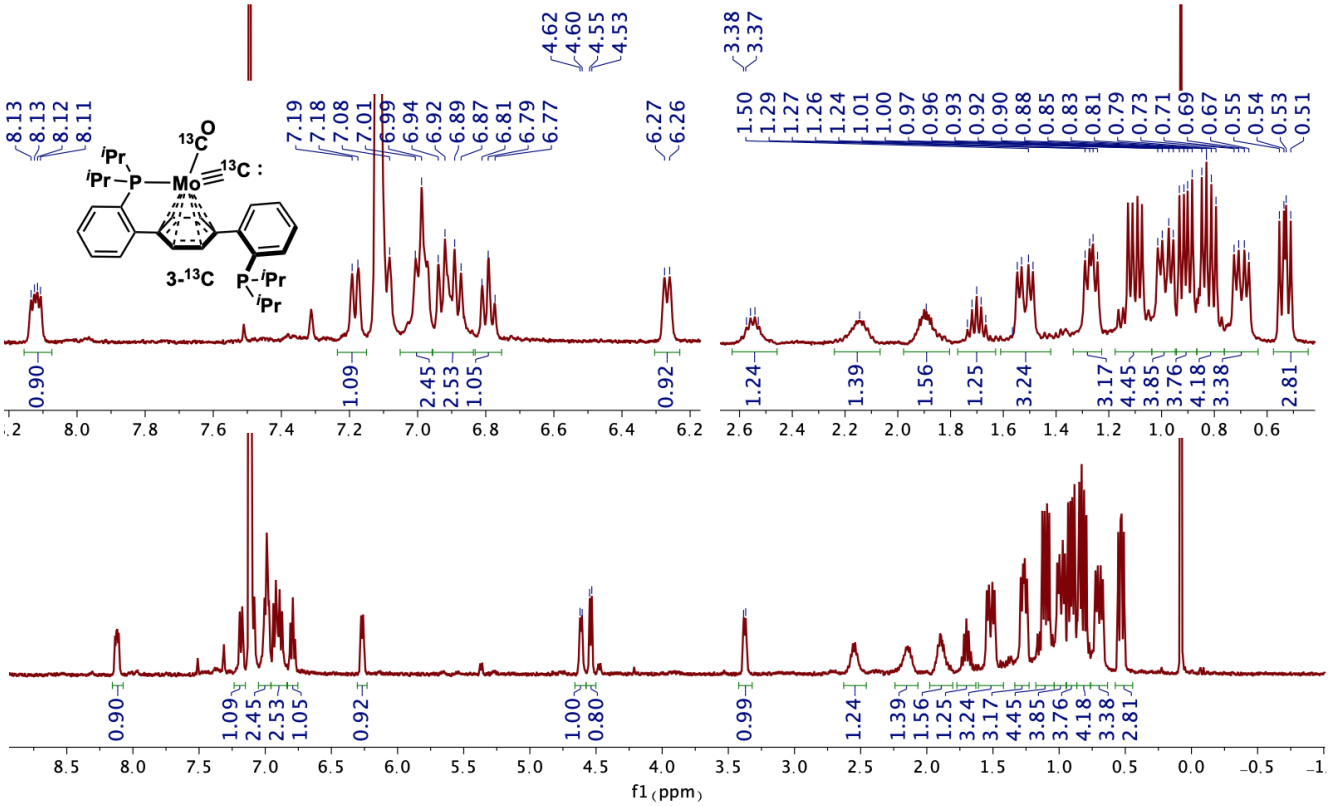


Figure S7—^{1}H NMR Spectrum (400 MHz, C_6D_6, 23 °C) of **3-^{13}C**. Insets magnify the crowded regions of the spectrum.

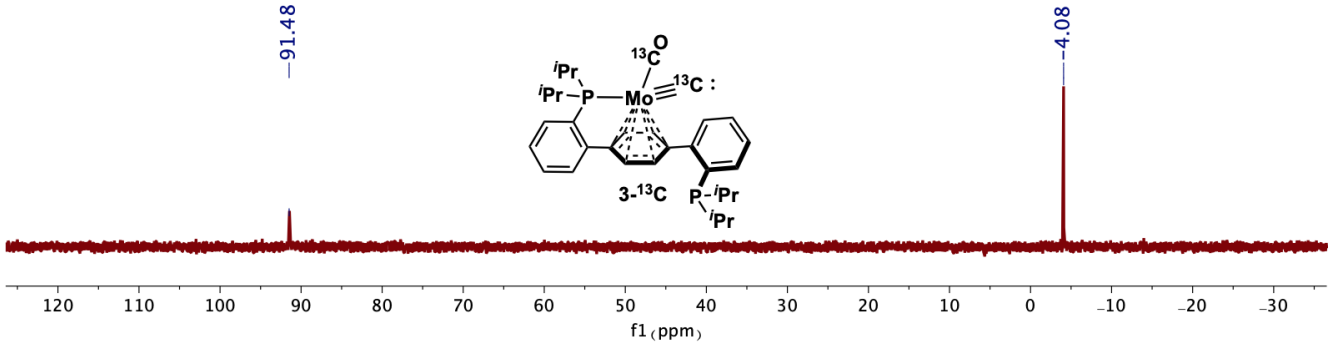


Figure S8—^{31}P{^{1}H} NMR spectrum (162 MHz, C_6D_6, 23 °C) of **3-^{13}C**.

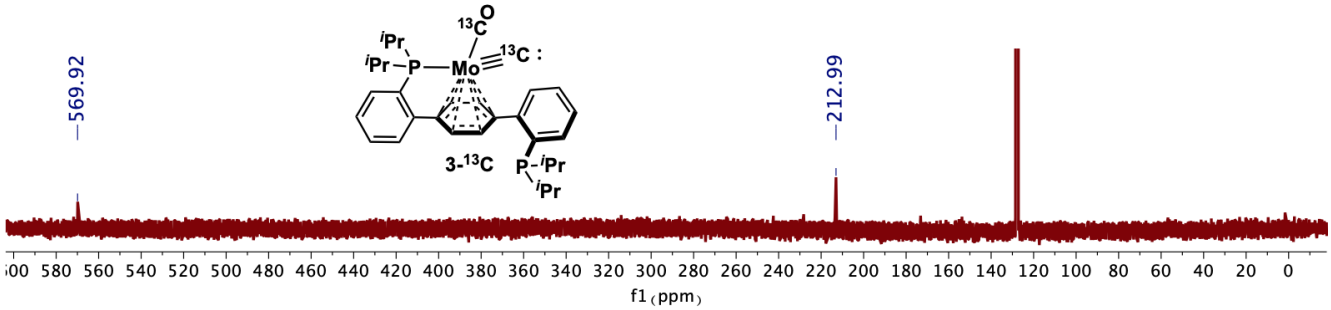
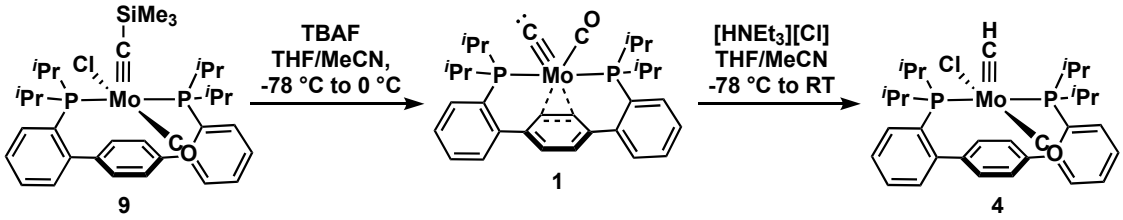


Figure S9—^{13}C{^{1}H} NMR spectrum (101 MHz, C_6D_6, 23 °C) of **3-^{13}C** showing key, ^{13}C-labelled resonances.

Sequential Proton & Hydride Addition to Carbide 1

Synthesis of Methylidyne **4**



A 300 mL Teflon-stoppered Schlenk tube was charged with **9** (2.03 g, 2.87 mmol), THF (125 mL), and a stir bar. The flask was sealed, attached to a Schlenk line, and cooled to -78 °C via submersion in a dry ice/acetone slush bath. With a heavy N_2 counterflow, the stopper was replaced with a septum. A dark red MeCN solution of anhydrous TBAF (4.31 mmol, 1.5 equiv) was added dropwise via syringe. The reaction mixture was allowed to warm to 0 °C, with stirring, and maintained at this temperature for 2 h. At this time, the flask was once again cooled to -78 °C and [$HNEt_3$][Cl] (1.185 g, 8.61 mmol, 3 equiv) was added in a single portion, as a solid, with a heavy N_2 counterflow. The vessel was sealed, shaken vigorously, and left to stir for 2 h while warming to room temperature. Volatile reaction components were removed under reduced pressure and the resulting residue was extracted with PhMe (5 x 50 mL) and filtered through a pad of Celite. The orange/red homogeneous filtrate was dried *in vacuo*, affording a red/orange residue. This residue was suspended in minimal THF (4 mL), and cooled to -35 °C for 12 h. The ensuing mixture was filtered through celite and the filtrate set aside. The filter cake was washed with C_6H_6 until the filtrate was colorless (*ca.* 100 mL). Lyophilization of the C_6H_6 filtrate under reduced pressure afforded **4** as an orange powder (1.50 g, 82%). ^{1}H NMR (300 MHz, C_6D_6, 23 °C) δ: 7.51 (s, 2H, central arene-*H*), 7.43-7.48 (br m, 2H, aryl-*H*), 7.31-7.36 (br m, 2H, aryl-*H*), 7.25 (s, 2H, central arene-*H*), 7.17-7.20 (br m, 4H, aryl-H; overlaps with the downfield edge of the C_6D_5H solvent residual), 5.08 (t, *J* = 3.44 Hz, 1H, Mo≡C*H*), 2.34-2.45 (m, 2H, C*H*(CH_3)$_2$), 2.21-2.34 (m, 2H, C*H*(CH_3)$_2$), 1.69-1.76 (m, 6H, CH(C*H*$_3$)$_2$), 1.36-1.43 (m, 6H, CH(C*H*$_3$)$_2$), 1.26-1.33 (m, 6H, CH(C*H*$_3$)$_2$), 1.06-1.12 (m, 6H, CH(C*H*$_3$)$_2$). ^{13}C{^{1}H} NMR (100.6 MHz, C_6D_6, 23 °C) δ: 282.34 (t, *J* = 18.3 Hz, Mo≡C*H*), 242.6 (t, *J* = 10.1 Hz, *C*O), 148.17 (t, *J* = 7.0 Hz, aryl-*C*), 138.47 (t, *J* = 2.5 Hz, aryl-*C*), 133.63 (t, *J* = 10.4 Hz, aryl-*C*), 132.45 (s, aryl-*C*), 129.59 (t, *J* = 2.5 Hz, aryl-*C*), 129.49 (s, aryl-*C*), 120.86 (s, aryl-*C*), 34.79 (t, *J* = 9.8 Hz, ^{i}Pr-*C*), 31.27 (t, *J* = 7.1 Hz, ^{i}Pr-*C*), 21.94 (t, *J* = 21.9 Hz, ^{i}Pr-*C*), 21.22 (s), 20.14 (t, *J* = 3.0 Hz. ^{i}Pr-*C*), 19.77 (s). ^{31}P{^{1}H} NMR (121 MHz, C_6D_6, 23 °C) δ: 40.21 (s). Anal. Calcd. for **4** $C_{32}H_{41}MoClOP_2$ (%): C, 60.53; H, 6.51. Found: 61.02; H, 6.60. FTIR (ATR, cm^{-1}): 1852 (s, C≡O).

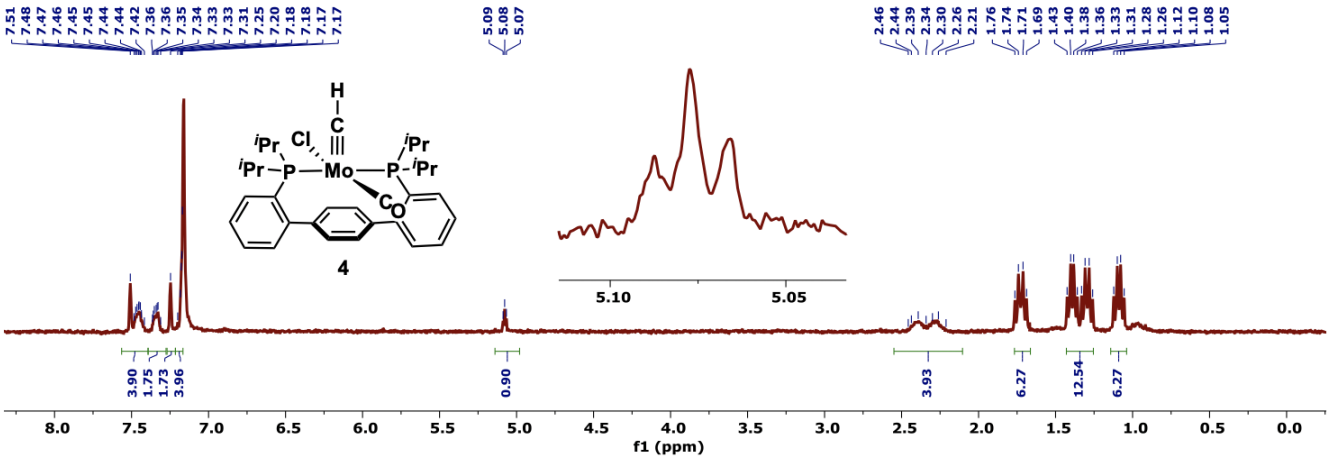


Figure S10—^{1}H NMR Spectrum (300 MHz, C_6D_6, 23 °C) of **4**. The inset shows an enlargement of the triplet corresponding to the methylidyne proton.

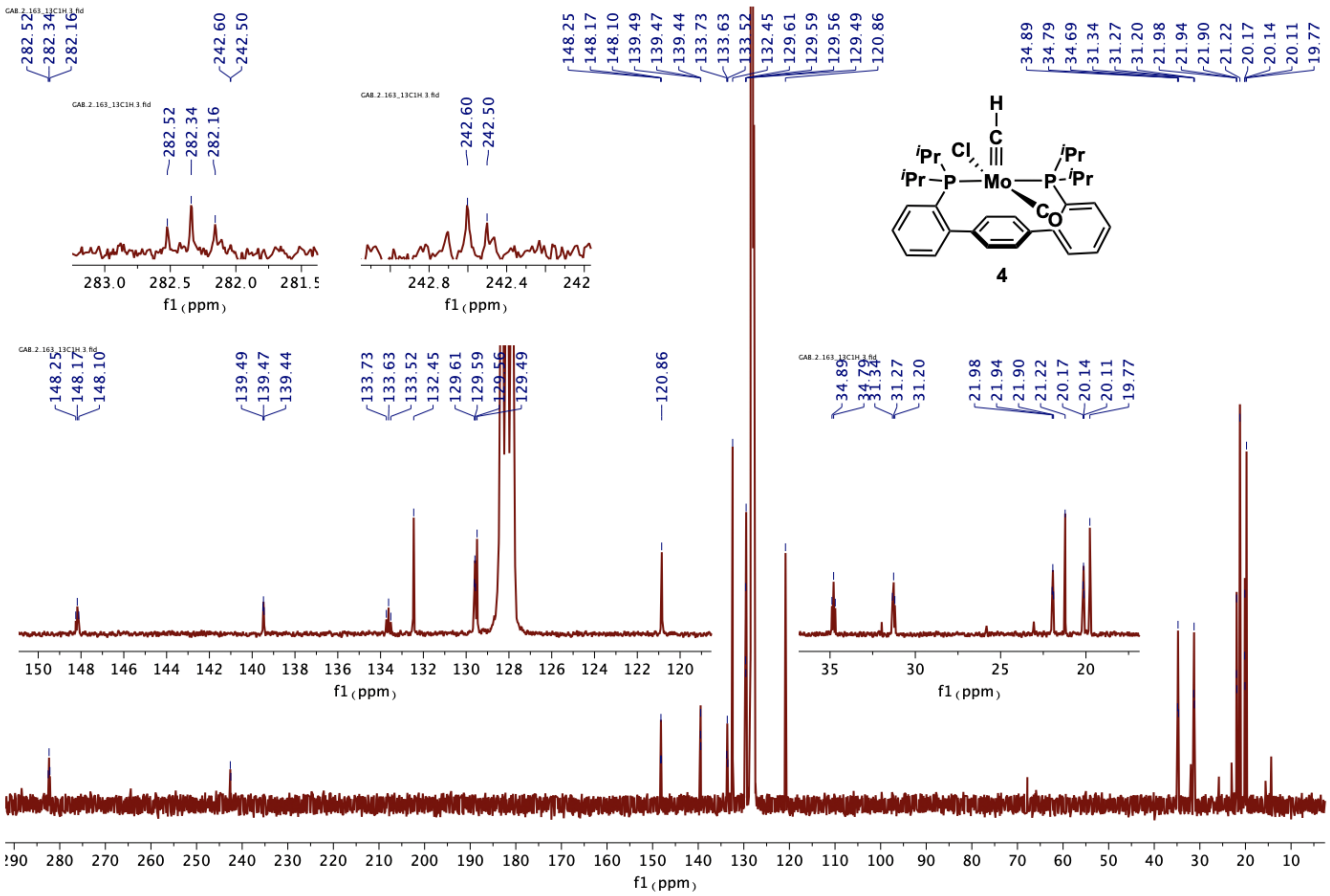


Figure S11—$^{13}C\{^{1}H\}$ NMR Spectrum (300 MHz, C_6D_6, 23 °C) of **4**. The insets magnify the methylidyne and CO resonances, and the more crowded regions of the spectrum.

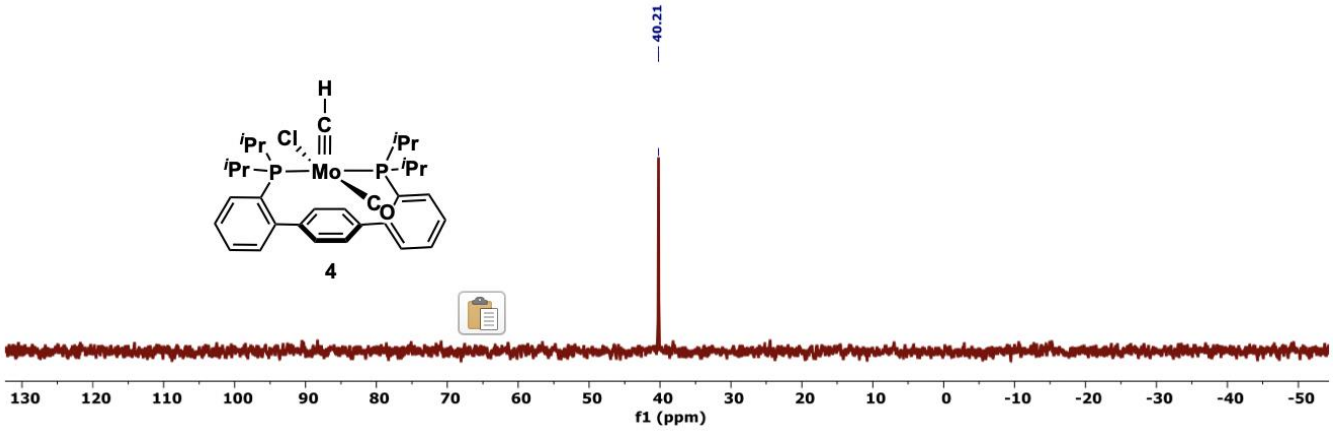


Figure S12—$^{31}P\{^{1}H\}$ NMR Spectrum (121 MHz, C_6D_6, 23 °C) of **4**.

Synthesis of **4-^{13}C**

4-^{13}C can be prepared analogously, starting from **9-^{13}C**. The ^{1}H NMR spectrum (300 MHz, C_6D_6, 23 °C) shows a 147.8 Hz ^{1}J(C,H) scalar coupling for the methylidyne proton, splitting it into a doublet of triplets. The enhanced resonances in the $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, C_6D_6, 23 °C) are 281.19 (br, Mo≡*C*H) and 241.41 (br, Mo-

*C*O); however, the ^{1}J(C,H) and ^{2}J(C,P) coupling is not resolved. The $^{31}P\{^{1}H\}$ NMR spectrum (121 MHz, C_6D_6, 23 °C) shows the well resolved ^{2}J(C,P) couplings to the methylidyne and carbonyl carbons: 18.3 and 10.0 Hz.

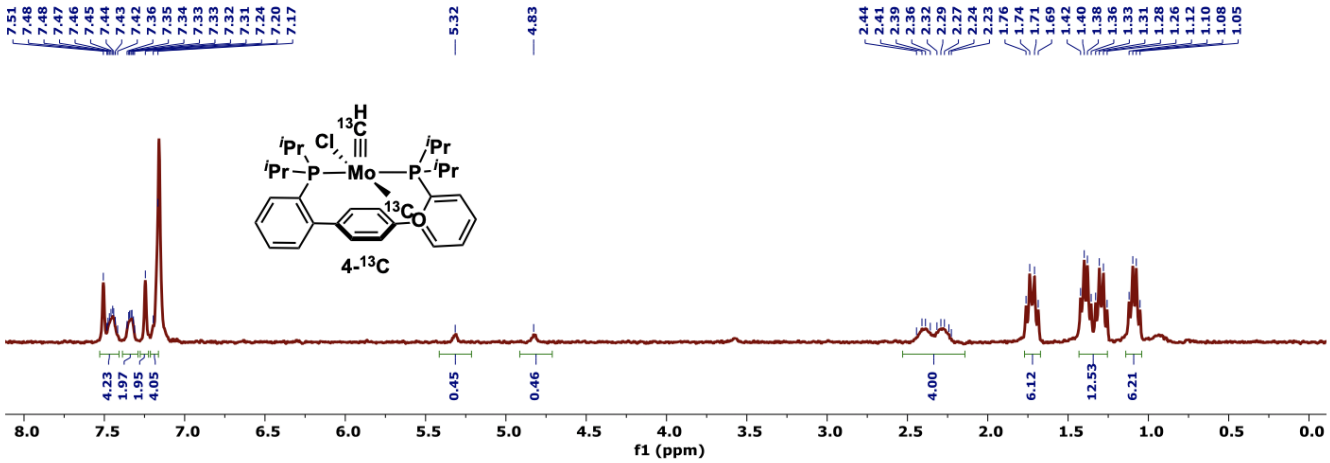


Figure S13—^{1}H NMR Spectrum (300 MHz, C_6D_6, 23 °C) of **4-^{13}C**. The methylidyne proton is split into a doublet centered at 5.08 ppm (^{1}J(C,H) = 147.21 Hz).

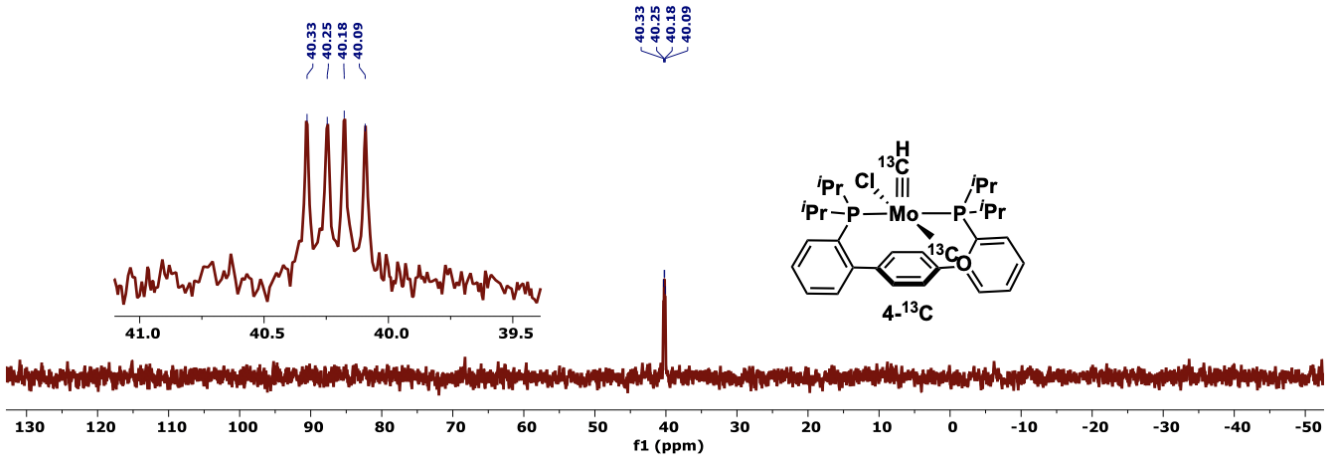


Figure S14—$^{31}P\{^{1}H\}$ NMR Spectrum (121 MHz, C_6D_6, 23 °C) of **4-^{13}C**. The inset shows the well resolved ^{2}J(C,P) couplings to the methylidyne and carbonyl carbons: 18.3 and 10.0 Hz.

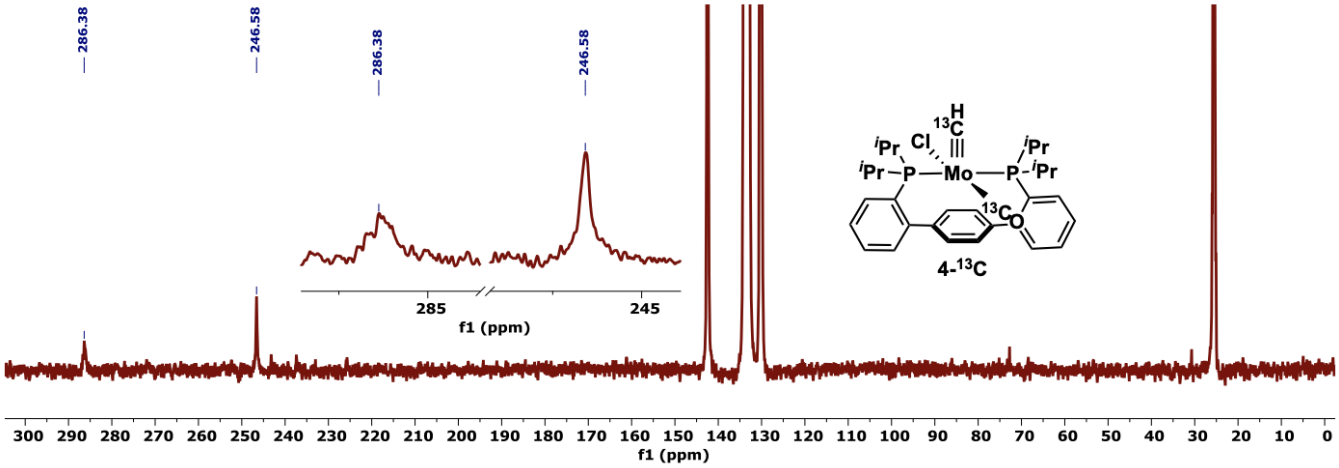
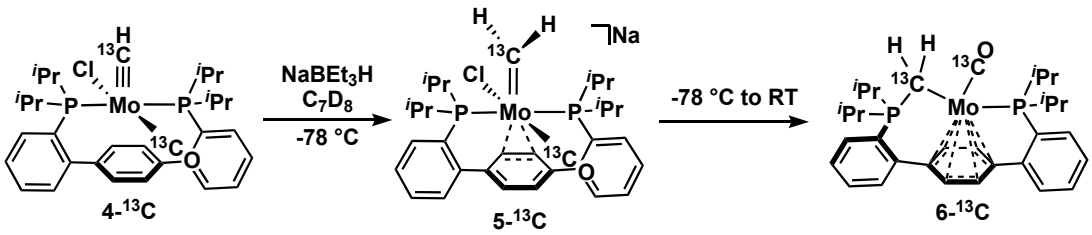


Figure S15—$^{13}C\{^{1}H\}$ NMR Spectrum (126 MHz, C_7D_8, -78 °C) of **4-^{13}C**. The inset shows the broad resonances of the isotopically enriched methylidyne (286.38 ppm) and carbonyl (246.58 ppm) carbon atoms.

*Addition of $NaBEt_3H$ to **4**—In Situ Formation of **5** and Synthesis of Phosphonium Ylide Complex **6***



For synthesis and characterization of non-labelled **6**, see below. A J. Young NMR tube was charged with an orange suspension of **4-^{13}C** (25 mg, 0.039 mmol) in C_7D_8. The tube was sealed and attached to a high vacuum manifold. The reaction was cooled to -78 °C in a dry ice/acetone bath and with a heavy Ar counterflow, a solution of $NaBEt_3H$ in PhMe (0.040 mL, 0.040 mmol) was added, resulting in an immediate darkening of the reaction mixture to brown. Low temperature multinuclear NMR spectroscopy (^{1}H, $^{31}P\{^{1}H\}$, $^{13}C\{^{1}H\}$, -80 °C) demonstrated quantitative conversion to methylidene **5-^{13}C**. Key data: ^{1}H NMR (500 MHz, C_7D_8, -80 °C): 15.03 (dd, J = 114.9, J = 13.3, Mo=C*H*H), 13.27 (d, J = 142.7, Mo=CH*H*). $^{13}C\{^{1}H\}$ NMR (126 MHz, C_7D_8, -80 °C): 297.23 (br s), 237.68 (br s). $^{31}P\{^{1}H\}$ NMR (202 MHz, C_7D_8, -80 °C): 52.07 (br s).

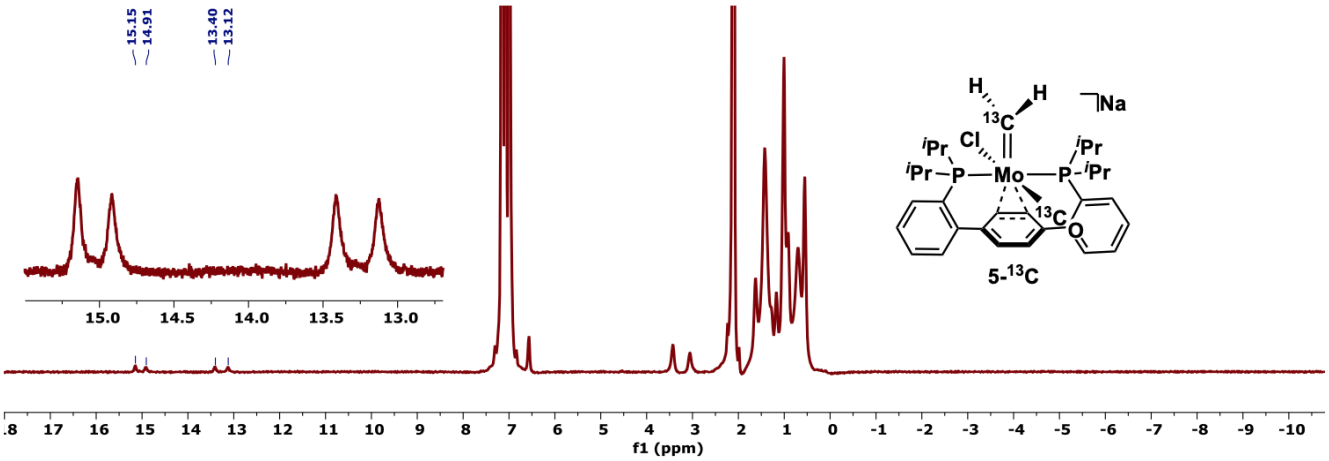


Figure S16—^{1}H NMR Spectrum (500 MHz, C_7D_8, -80 °C) of **5-^{13}C**. The inset shows an enlargement of the downfield resonances assigned to the methylidene protons.

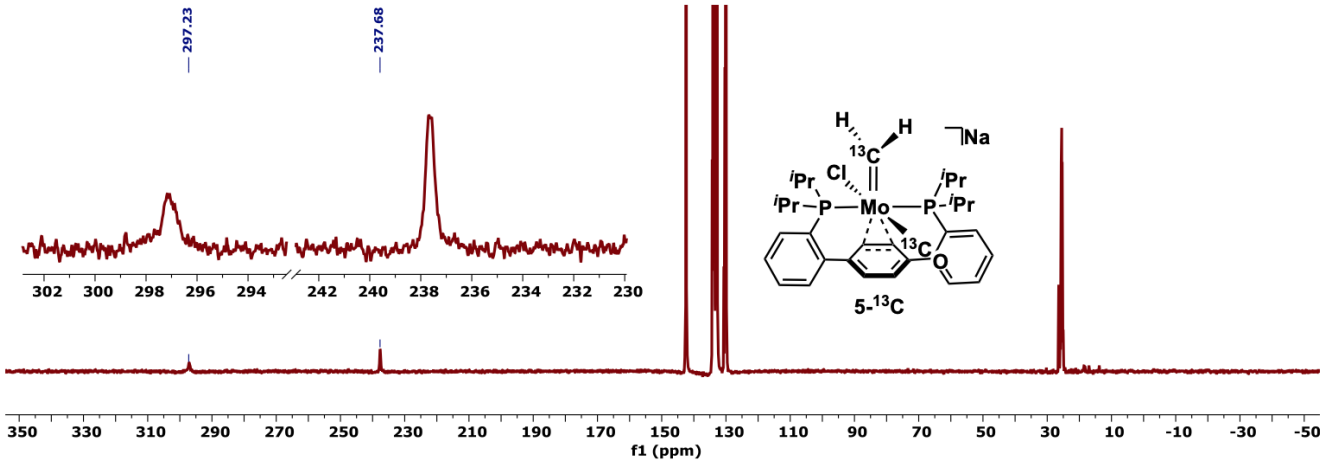


Figure S17—^{13}C{^{1}H} NMR Spectrum (126 MHz, C_7D_8, -80 °C) of **5-^{13}C**. The inset shows an enlargement of the isotopically enriched methylidene and carbonyl carbon signals.

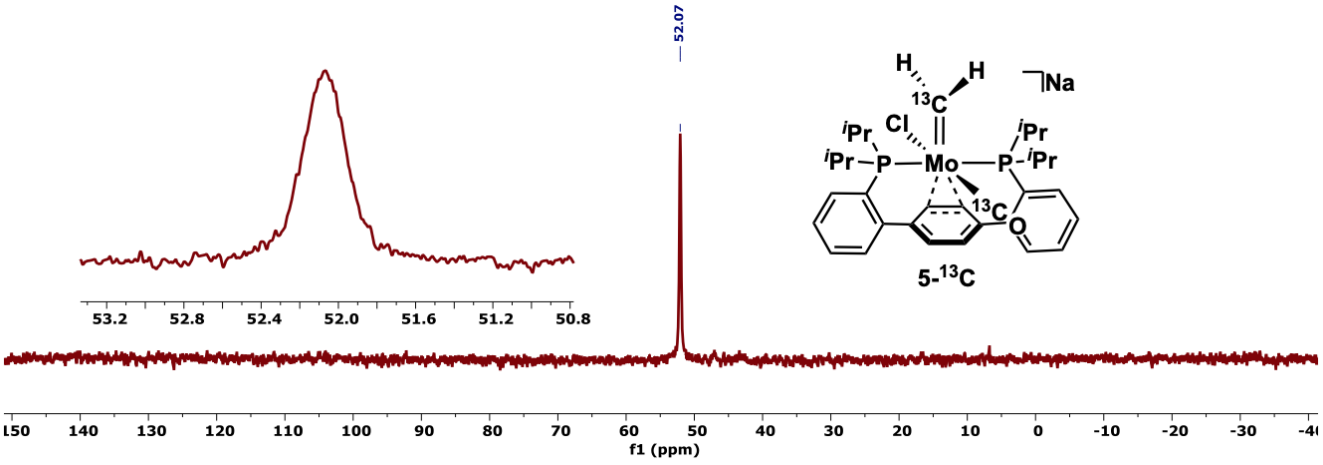


Figure S18—^{31}P{^{1}H} NMR spectrum (202 MHz, C_7D_8, -80 °C) of **5-^{13}C**.

The tube was warmed incrementally in the spectrometer probe, showing the growth of a new species at *ca.* -10 °C (Fig. S15). Compound **6-^{13}C** persisted at room temperature, facilitating its isolation. The J. Young tube was returned to the glovebox and the contents transferred to a 20 mL vial charged with a stir bar. The reaction volatiles were removed under reduced pressure; the resulting residue extracted with benzene (*ca.* 3 mL) and the extract filtered through a Celite plug. The filtrate was lyophilized to afford **6-^{13}C** as an orange/brown powder (18 mg, 0.029 mmol, 77%). ^{1}H NMR (600 MHz, C_6D_6, 23 °C) δ: 7.63 (ddd, *J* = 7.7, 2.2, & 1.4 Hz, 1H, aryl-*H*), 7.51 (ddd, *J* = 7.7, 4.5, 1.4 Hz, 1H, aryl-*H*), 7.32 – 7.26 (m, 1H, aryl-*H*), 7.11 (app tt, *J* = 7.4, 1.3 Hz, 1H, aryl-*H*), 7.08 (app tt, *J* = 7.2, 1.4 Hz, 1H, aryl-*H*), 6.96 (app tt, *J* = 7.6, 1.4 Hz, 1H, aryl-*H*), 6.85 – 6.81 (m, 1H, aryl-*H*), 6.71 (ddd, *J* = 9.4, 7.9, 1.3 Hz, 1H, aryl-*H*), 4.64 (dd, *J* = 4.9, 1.4 Hz, 1H, central arene-*H*), 4.52 – 4.48 (m, 1H, central arene-*H*), 4.24 (d, *J* = 4.3 Hz, 1H, central arene-*H*), 3.93 (ddd, *J* = 6.5, 2.6, 1.4 Hz, 1H, central arene-*H*), 2.70 – 2.64 (m, 1H, C*H*$(CH_3)_2$), 2.61 – 2.54 (m, 1H, C*H*$(CH_3)_2$), 2.54 – 2.47 (m, 1H, C*H*$(CH_3)_2$), 1.86 –1.77 (m, 1H, C*H*$(CH_3)_2$), 1.42 – 1.33 (m, 3H, CH(C*H*$_3)_2$), 1.31 – 1.27 (m, 3H, CH(C*H*$_3)_2$), 1.27 – 1.23 (m, 3H, CH(C*H*$_3)_2$), 1.20 – 1.16 (m, 6H, CH(C*H*$_3)_2$), 1.00 (dt, *J* = 127.0 Hz & 11.4 Hz, 1H, PC*H*$_2$Mo), 0.78 – 0.74 (m, 6H, CH(C*H*$_3)_2$), 0.64 (ddd, *J* = 128.6, 12.1, & 2.7 Hz, 1H, PC*H*$_2$Mo), 0.61– 0.58 (m, 3H, CH(C*H*$_3)_2$). ^{13}C{^{1}H} NMR (125 MHz, C_6D_6, 23 °C) δ: 251.88 (app dt, *J* = 15.3, 2.2 Hz), 150.77 (s, aryl-*C*), 150.49 (s, aryl-*C*), 150.22 (s, aryl-*C*), 150.18 (s, aryl-*C*), 132.39 (d, *J* = 5.3 Hz, aryl-*C*), 131.65 (d, *J* = 9.6 Hz, aryl-*C*), 130.06 (d, *J* = 2.1 Hz, aryl-*C*), 128.34 (s, aryl-*C*), 128.22 (s, aryl-*C*), 127.74 (aryl-*C*, coincides with C_6D_6 solvent residual but corroborated via 2D NMR spectroscopy), 126.42 (d, *J* = 4.0 Hz, aryl-*C*), 124.67 (d, *J* = 10.7 Hz, aryl-*C*), 105.37 (s, central arene-*C*), 96.86 (s, central arene-*C*), 81.02 (d, *J* = 2.8 Hz, central arene-*C*), 80.26-80.38 (m, central arene-*C*), 78.49 (s, central arene-*C*), 72.33 (s, central arene-*C*), 28.56 (d, *J* = 18.0 Hz, *C*H$(CH_3)_2$), 27.72 (d, *J* = 8.8 Hz, *C*H$(CH_3)_2$), 26.33 (dd, J = 51.7, 3.4 Hz, *C*H$(CH_3)_2$), 22.71 (d, *J* = 34.2 Hz, *C*H$(CH_3)_2$), 19.72 (d, *J* = 9.4 Hz, CH(*C*H$_3)_2$), 19.46 (d, *J* = 5.4 Hz, CH(*C*H$_3)_2$), 19.22 (d, J = 6.48 Hz, CH(*C*H$_3)_2$), 18.46 (s, CH(*C*H$_3)_2$), 18.14 (d, J = 2.5 Hz, CH(*C*H$_3)_2$), 16.42 (s, CH(*C*H$_3)_2$), 16.16 (d, J = 2.8 Hz, CH(*C*H$_3)_2$), 15.91 (d, J = 1.6 Hz, CH(*C*H$_3)_2$), -34.87 (ddd, *J* = 21.8, 6.2, 2.2 Hz, P*C*H$_2$Mo). ^{31}P{^{1}H} NMR (162 MHz, C_6D_6, 23 °C) δ: 84.68 (app td, $^{3}J_{PP}$ = 16.5 Hz, $^{2}J_{PC}$ = 6.0 Hz, Mo-*P*), 47.41 (dd, $^{1}J_{PC}$ = 21.9 Hz, $^{3}J_{PP}$ = 17.0 Hz, *P*CH$_2$Mo).

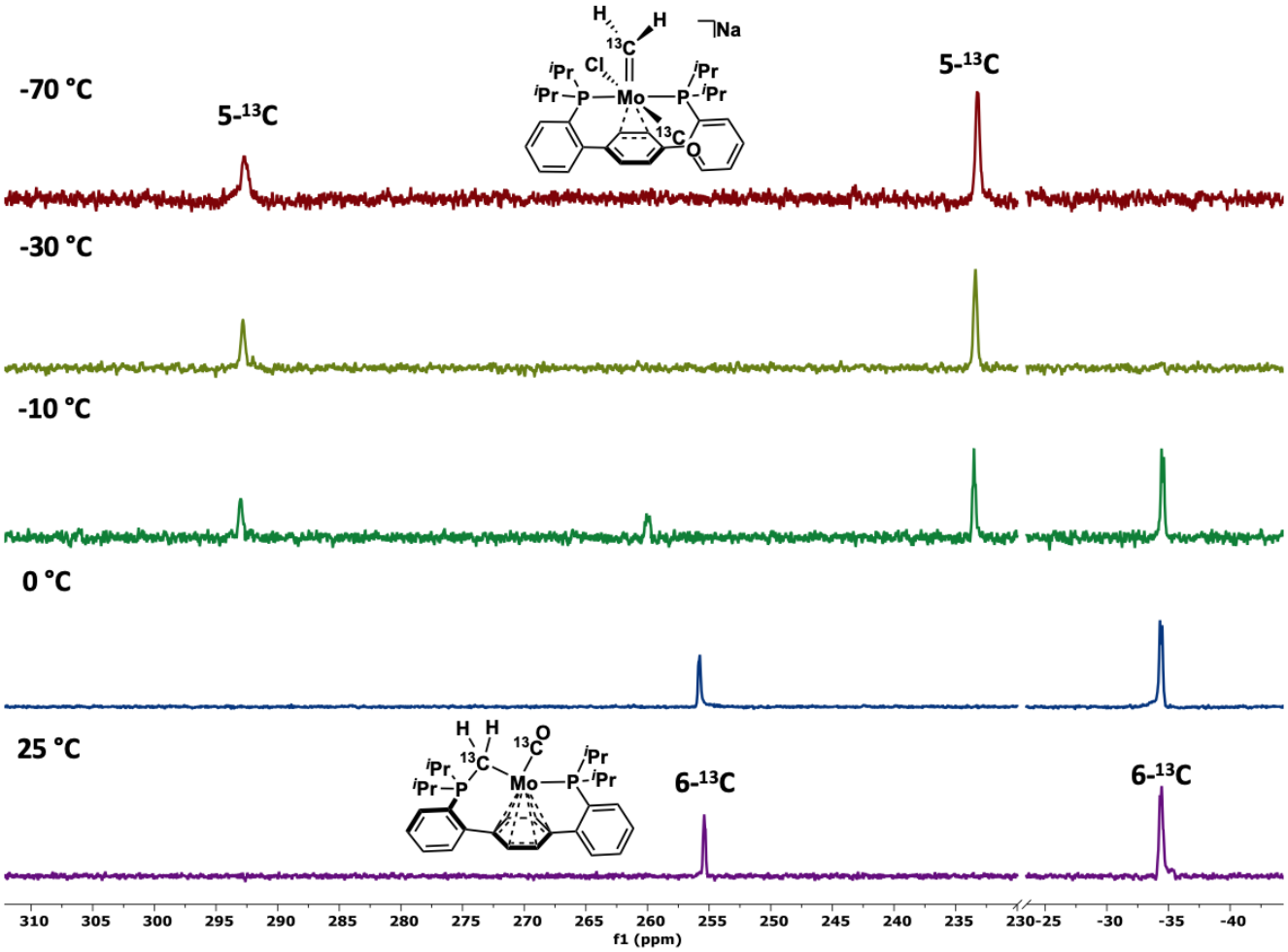


Figure S19—Variable temperature $^{13}C\{^{1}H\}$ (126 MHz, THF, -50 °C) spectra of methylidene complex **5-^{13}C** (top). Upon warming, clean conversion to **6-^{13}C** is observed (top to bottom).

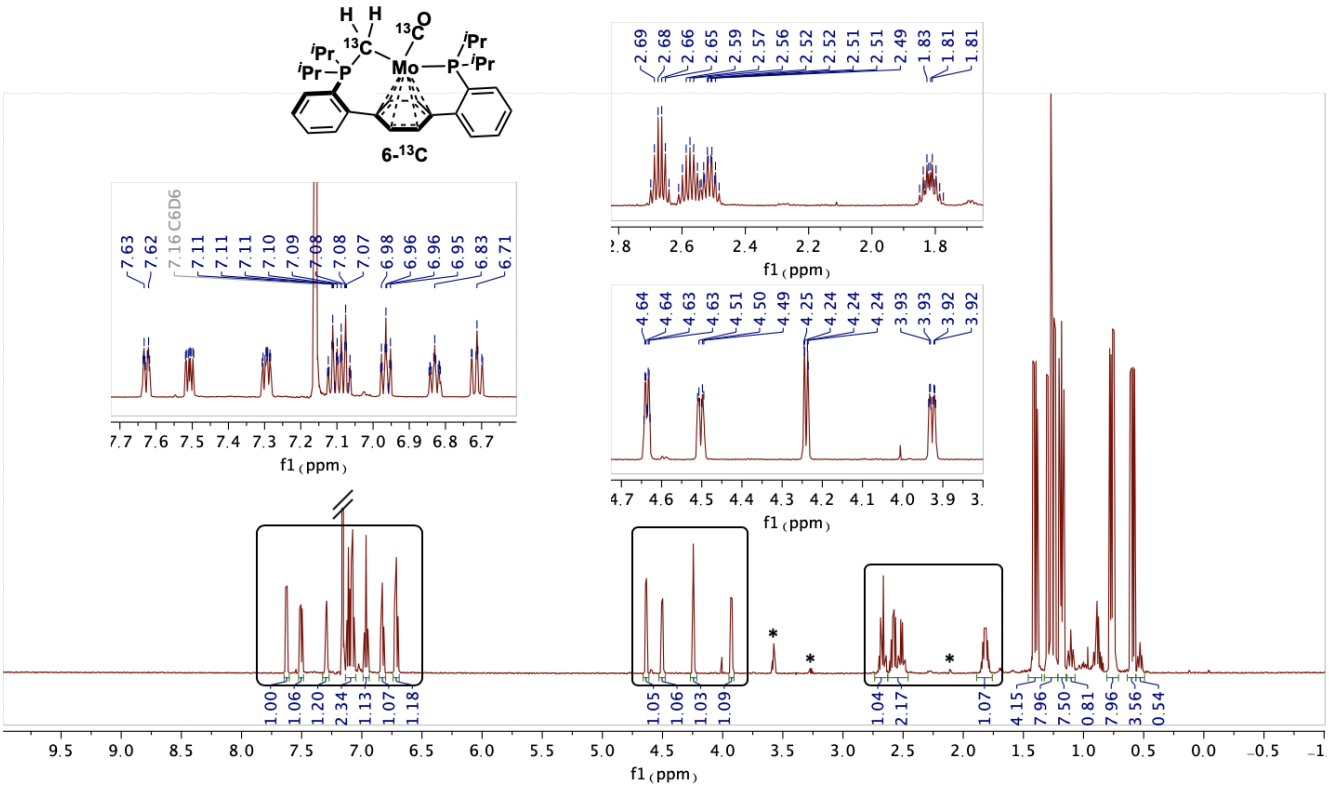


Figure S20—^{1}H NMR spectrum (600 MHz, C_6D_6, 23 °C) of **6-^{13}C**. The insets magnify the key aromatic and methine signals. (*) Denotes residual solvents (THF, Et_2O, toluene).

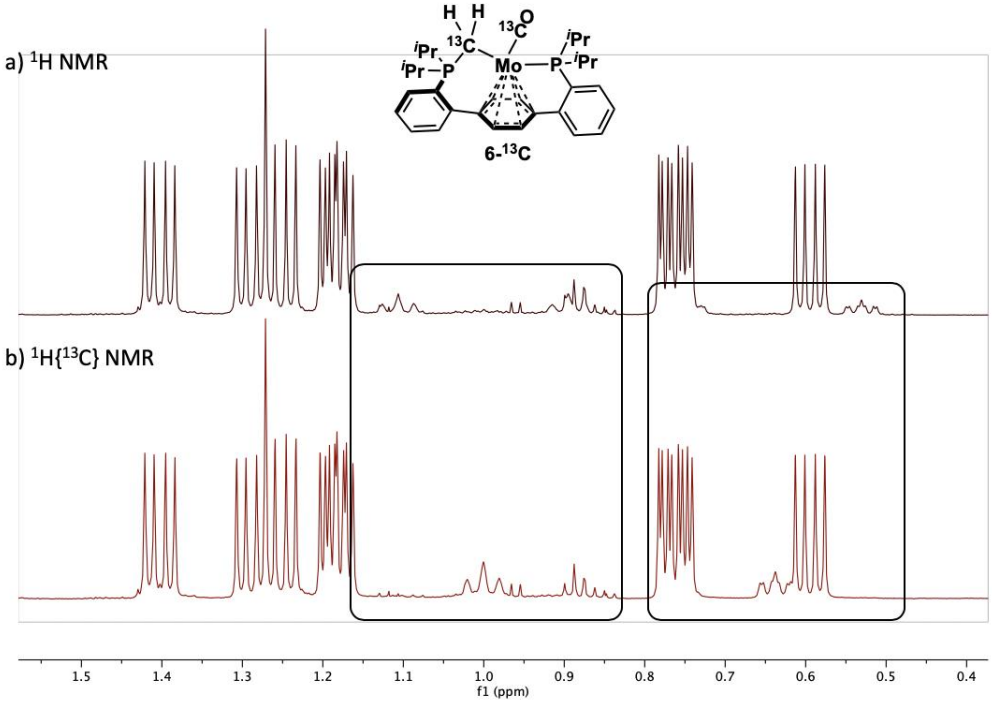


Figure S21—(a) ^{1}H and (b) ^{1}H{^{13}C} NMR spectra (600 MHz, C_6D_6, 23 °C) of **6-^{13}C** showing resolution of the two PCH_2 doublets of triplets into triplets on ^{13}C decoupling.

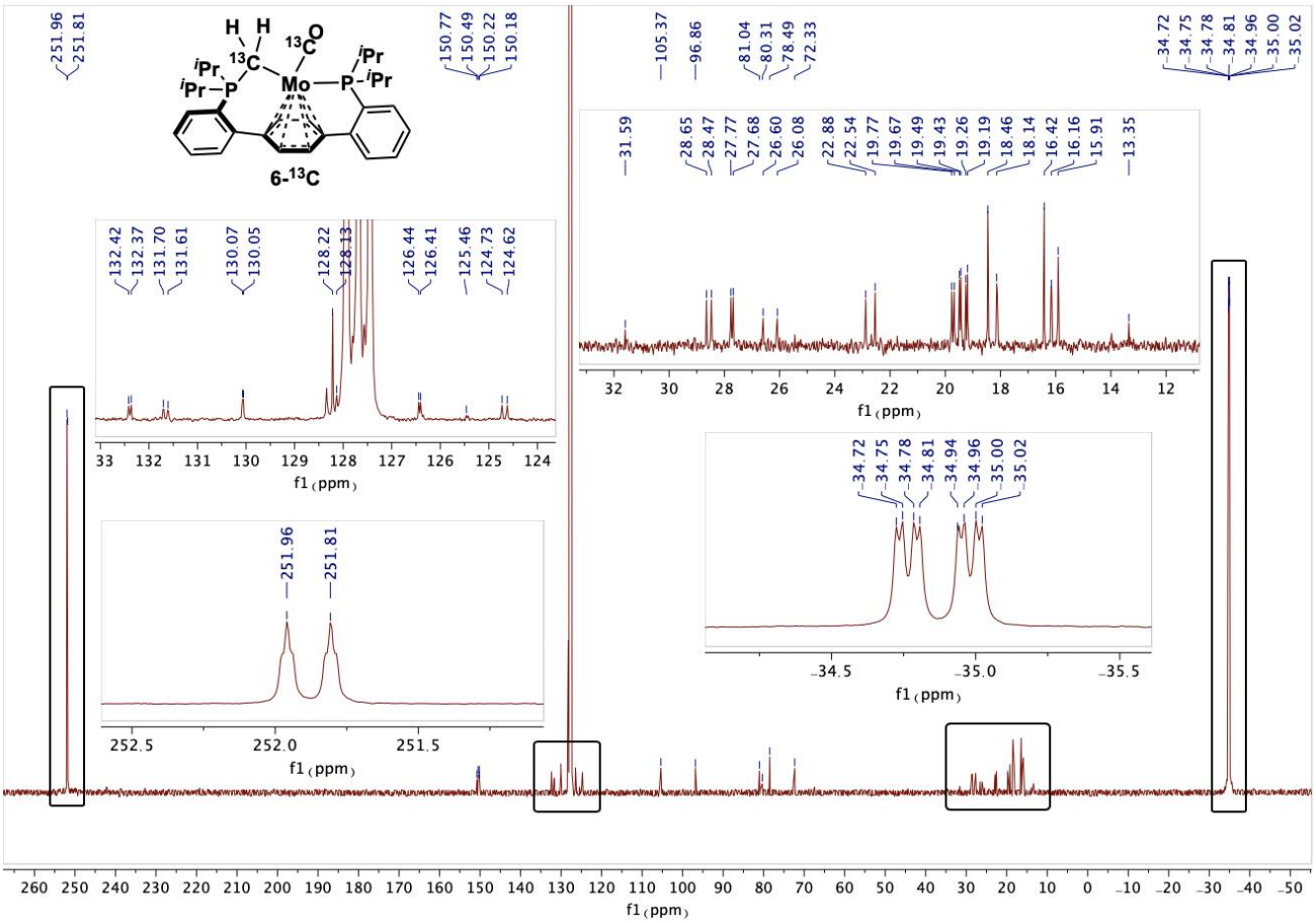


Figure S22—$^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, C_6D_6, 23 °C) of **6-^{13}C**. The insets magnify the isotopically enriched CO (bottom left) and methylene (bottom right) carbon resonances, and the more crowded regions of the spectrum.

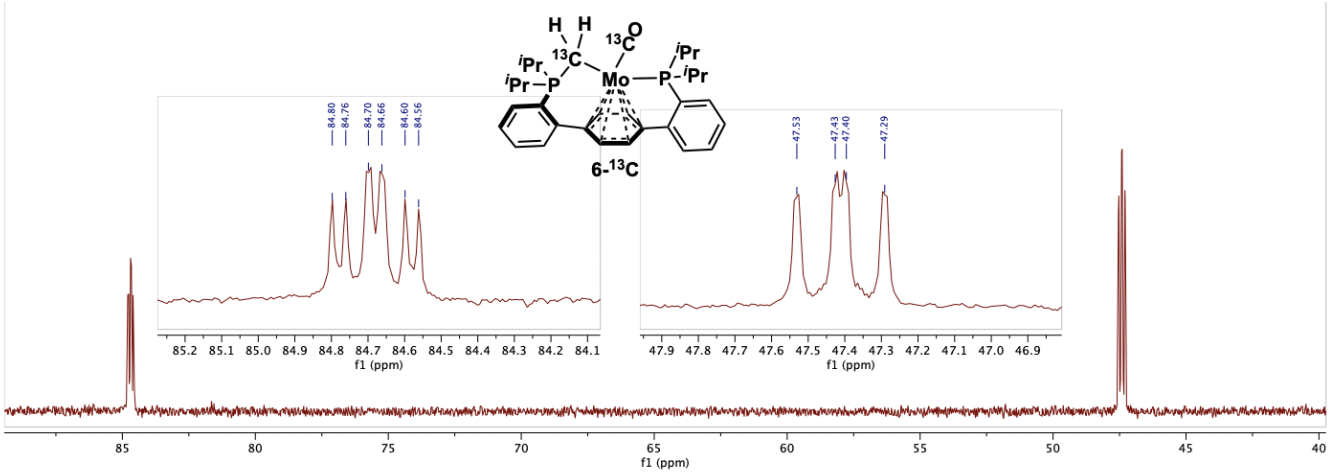


Figure S23—$^{31}P\{^{1}H\}$ NMR spectrum (126 MHz, C_6D_6, 23 °C) of **6-^{13}C**. The insets show the well resolved *J*(P,P) and *J*(P,C) coupling couplings.

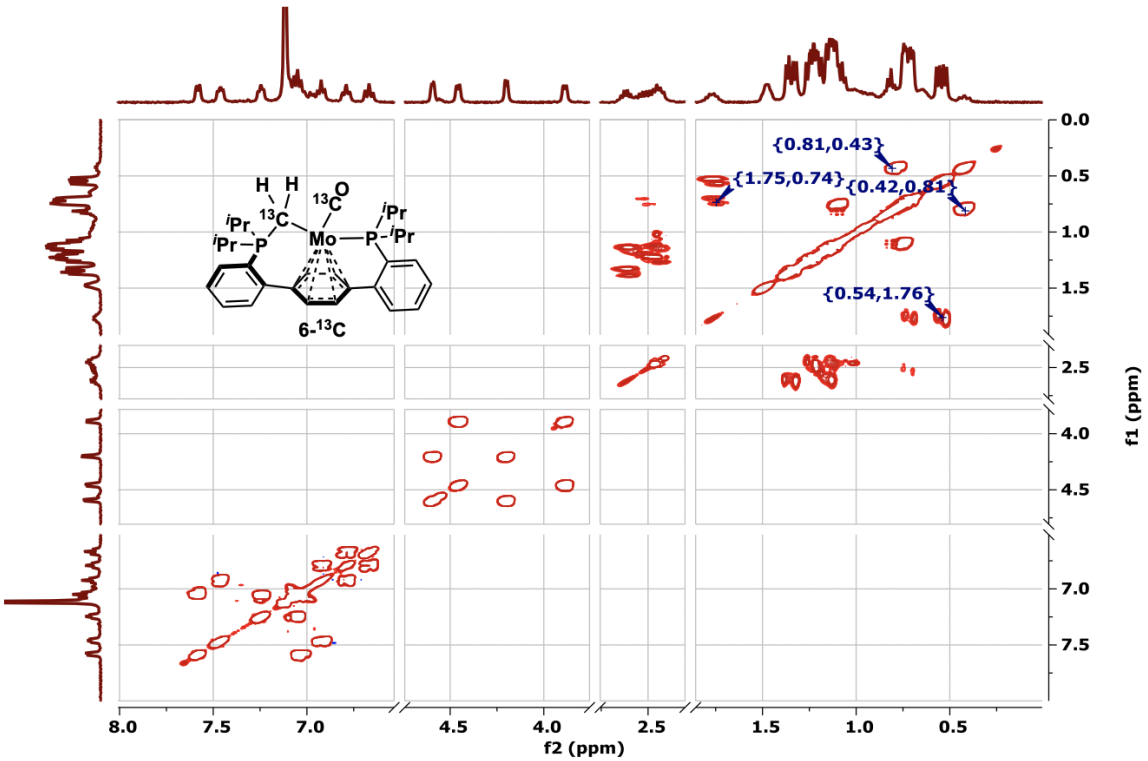


Figure S24—Partial $^{1}H/^{1}H$ COSY NMR spectrum (400 MHz, C_6D_6, 23 °C) of **6-^{13}C**. Cross-peaks critical to the assignment of the inserted methylene and isopropyl methine (of the methylene-bound phosphorous) are labeled.

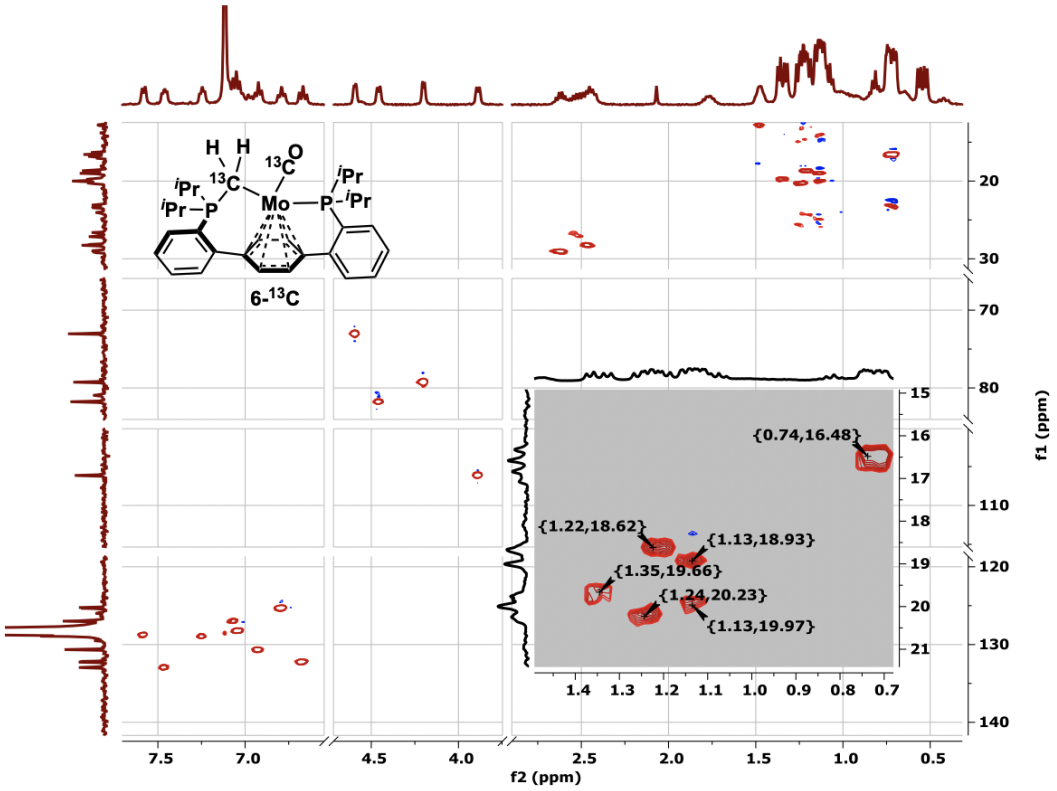


Figure S25—Partial $^{1}H/^{13}C$ HSQC NMR spectrum (400/101 MHz, C_6D_6, 23 °C) of **6-^{13}C**. The labeled crosspeaks aided in the assignment of the isopropyl methine and methyl carbon resonances. The grey inset shows an enlargement of the aliphatic region.

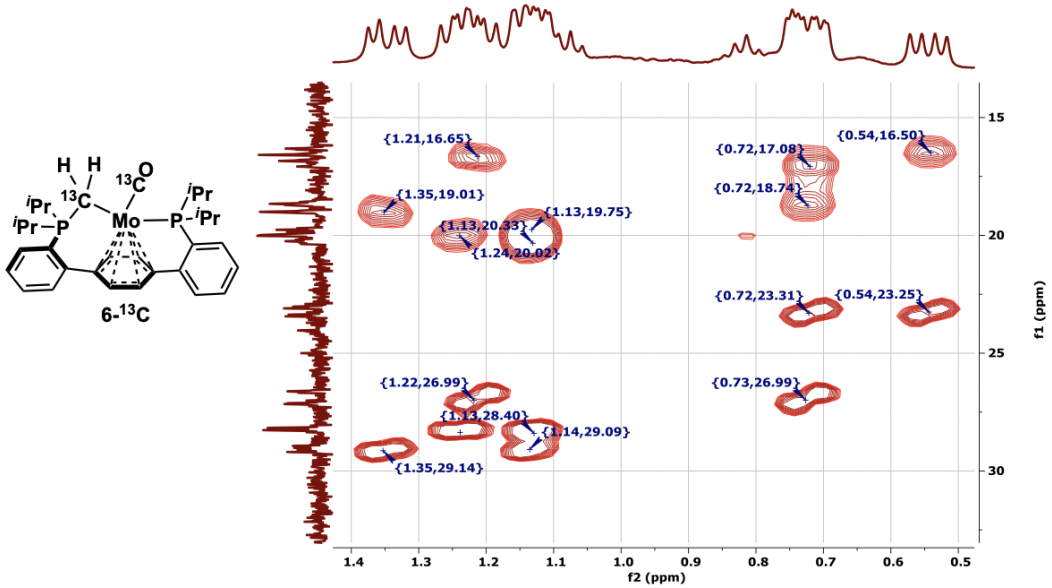


Figure S26— Partial $^{1}H/^{13}C$ HMBC NMR spectrum (400/101 MHz, C_6D_6, 23 °C) of **6-^{13}C**. The labeled crosspeaks aided in the assignment of the isopropyl methine and methyl carbon resonances.

Non-labelled **6** can be prepared analogously, starting from **4**. ^{1}H NMR (400 MHz, C_6D_6, 23 °C): 7.65 – 7.61 (m, 1H, aryl-*H*), 7.53 – 7.48 (m, 1H, aryl-*H*), 7.32 – 7.26 (m, 1H, aryl-*H*), 7.15 – 7.00 (m, 2H, aryl-*H*), 6.96 (app t, *J* =

7.6 Hz, 1H, aryl-*H*), 6.86 – 6.71 (m, 1H, aryl-*H*), 6.71 (m, 1H, aryl-*H*), 4.64 (app d, *J* = 4.9, 1H, central arene-*H*), 4.50 (app d, *J* = 6.6 Hz, 1H, central arene-*H*), 4.24 (d, *J* = 4.3 Hz, 1H, central arene-*H*), 3.93 (app d, *J* = 6.5 Hz, 1H, central arene-*H*), 2.73 – 2.61 (m, 1H, C*H*(CH_3)$_2$), 2.62 – 2.37 (m, 2H, C*H*(CH_3)$_2$), 1.87 – 1.75 (m, 1H, C*H*(CH_3)$_2$), 1.40 (app dd, *J* = 15.7 Hz, *J* = 7.0 Hz, 3H, CH(C*H*$_3$)$_2$), 1.33 – 1.13 (m, 12 H, CH(C*H*$_3$)$_2$), 1.04 – 0.94 (overlapping m, 1H, PC*H*$_2$Mo), 0.82 – 0.72 (m, 6H, CH(C*H*$_3$)$_2$), 0.68 – 0.55 (overlapping m, 4H, PC*H*$_2$Mo and CH(C*H*$_3$)$_2$). $^{31}P\{^1H\}$ NMR (162 MHz, C_6D_6, 23 °C) δ: 84.68 (d, $^3J_{PP}$ = 16.9 Hz, Mo-*P*), 47.43 (d, $^3J_{PP}$ = 17.0 Hz, *P*CH_2Mo). FTIR (ATR, cm^{-1}): 1723 (C≡O). Single crystals of **6** were grown from via vapor diffusion of pentane into toluene at –35 °C. A single-crystal XRD study corroborated the proposed structure of **6**.

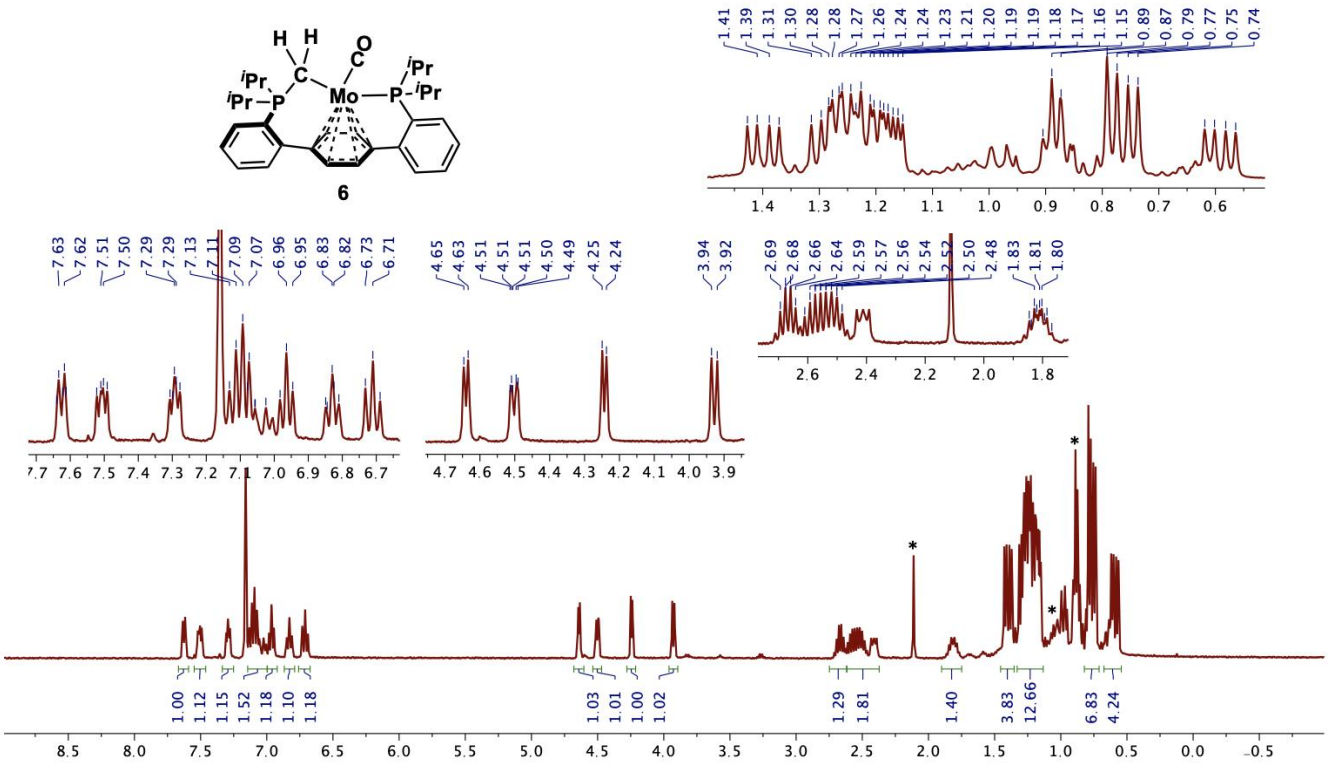


Figure S27—^1H NMR spectrum (400 MHz, C_6D_6, 23 °C) of **6**. The insets magnify the key regions of the spectrum. (*) Denotes residual solvents (hexanes, toluene).

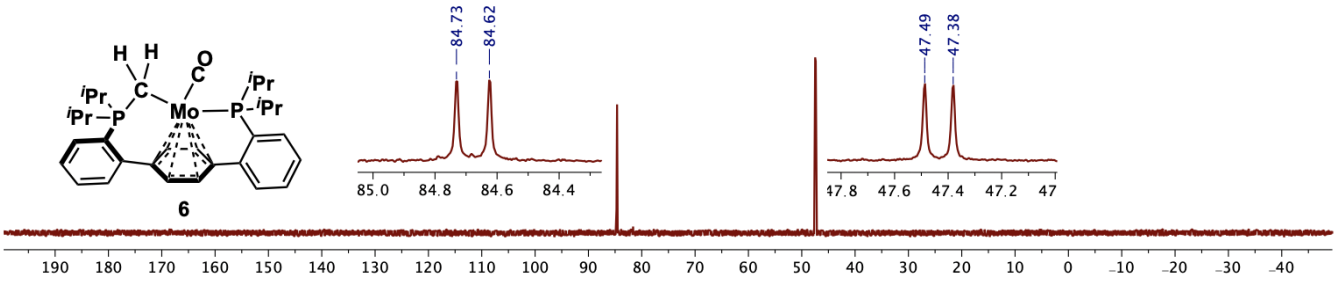
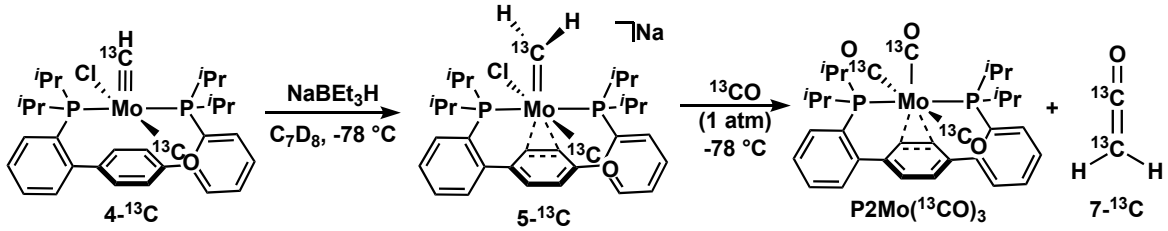


Figure S28—$^{31}P\{^1H\}$ NMR spectrum (126 MHz, C_6D_6, 23 °C) of **6**. The insets show the well resolved $^3J_{PP}$ couplings.

*CO-Promoted Ethenone Formation From **5-^{13}C***



A J. Young NMR tube was charged with an orange suspension of **4-^{13}C** (25 mg, 0.039 mmol) in C_7D_8. The tube was sealed and attached to a high vacuum manifold. The reaction was cooled to -78 °C in a dry ice/acetone bath and with a heavy Ar counterflow, a solution of $NaBEt_3H$ in PhMe (0.040 mL, 0.040 mmol) was added, resulting in an immediate darkening of the reaction mixture to brown. Low temperature multinuclear NMR spectroscopy (^{1}H, ^{31}P{^{1}H}, ^{13}C{^{1}H}, -78 °C) demonstrated quantitative conversion to methylidene **5** (Fig. S23, A). The J. Young tube was carefully removed from the NMR probe and returned to the -78 °C slush bath. Following attachment to a high vacuum manifold, the reaction was degassed via three freeze pump thaw cycles (thawing to -78 °C). The headspace was backfilled with ^{13}CO (1 atm) at -78 °C, resulting in a rapid lightening of the reaction mixture to bright orange as the gas diffused down the sample. The sample was returned to the -78 °C NMR probe and analyzed by ^{1}H, ^{31}P{^{1}H}, and ^{13}C{^{1}H} NMR spectroscopies (Fig. S23, B-C). Complete consumption of intermediate **5** was observed, concomitant with formation of the previously characterized tricarbonyl complex **P2Mo(**^{13}**CO)$_3$**.[9] The ^{13}C{^{1}H} NMR spectrum showed coupling doublets at 154.69 and 83.90 ppm (^1J(C,C) = 76.1 Hz), which may be consistent with an ethenone borane adduct. To further support ethenone formation, chemical trapping experiments were conducted.

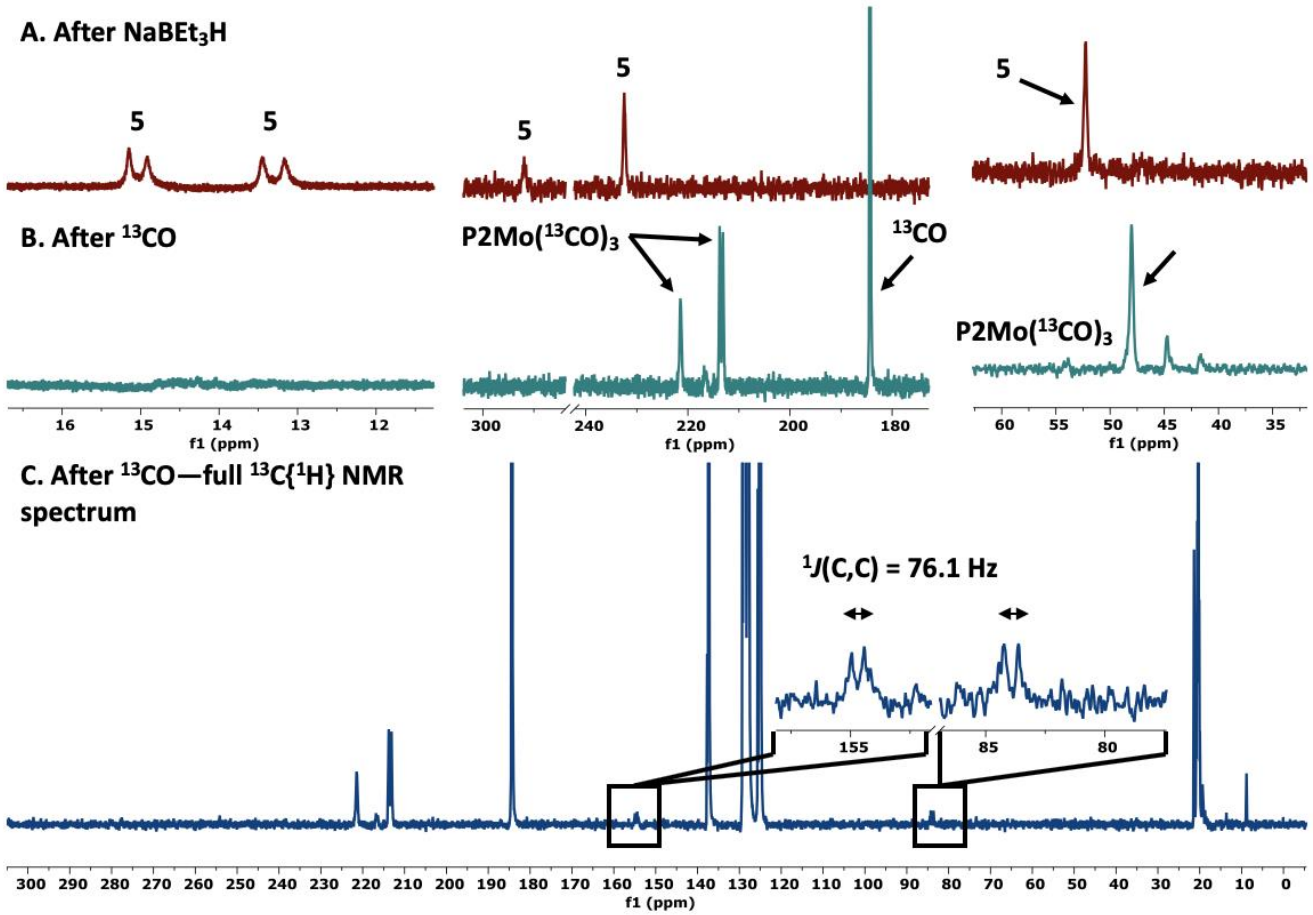
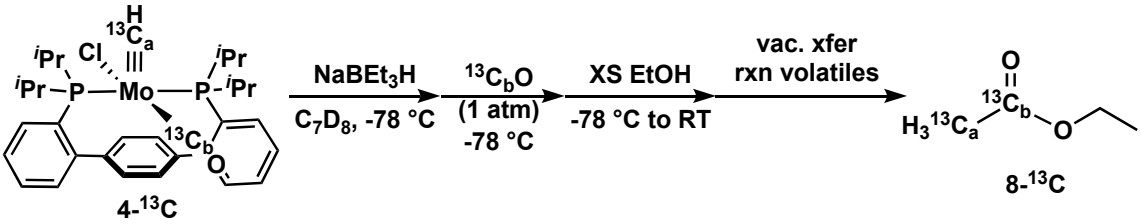


Figure S29—^{1}H (500 MHz), ^{13}C{^{1}H} (126 MHz), and ^{31}P{^{1}H} (202 MHz) NMR spectra (all C_7D_8, -78 °C) following the sequential addition of $NaBEt_3H$ (A) and ^{13}CO (B) to **4**. The enlargement (C) shows coupling doublets (154.69 and 83.90 ppm, ^{1}J(C,C) = 76.1 Hz) suggestive of ethenone-borane adduct formation.



Following the procedure outlined above, a solution of **4-^{13}C** (0.039 mmol) in C_7D_8 (0.5 mL) was prepared. The sample was degassed and backfilled with ^{13}CO, as before. Following the color change to bright orange, the reaction was frozen in liquid nitrogen. EtOH (*ca.* 0.1 mL) was admitted via vacuum transfer. The sample was carefully thawed and mixed thoroughly. At this point, the tube was appended to a transfer bridge and the reaction volatiles were vacuum transferred to a second, empty J. Young tube cooled with liquid nitrogen. Following complete transfer of the solvent, the receiving tube was thawed, affording a colorless solution. During the thawing process, the J. Young tube cracked, but the reaction solution was successfully collected in a 20 mL scintillation vial and transferred to an NMR tube. ^{13}C{^{1}H} NMR spectroscopy of this solution showed spectral features consistent with EtOAc-$^{13}C_2$, derived from the reaction of ^{13}C enriched ethenone with EtOH[10-11] (Note: the acetone impurity observed in the spectrum was introduced when the thawing sample tube broke; acetone was being used to warm the sides of the tube). The methyl carbon of EtOAc in C_7D_8 (20.46 ppm)[8] overlaps with the methyl group of the solvent. A selective decoupling experiment centered at 170.24 ppm (**10-^{13}C**, carbon C_b), substantiates the formation of **10-^{13}C**, collapsing the C_a doublet (Fig. S23, B).

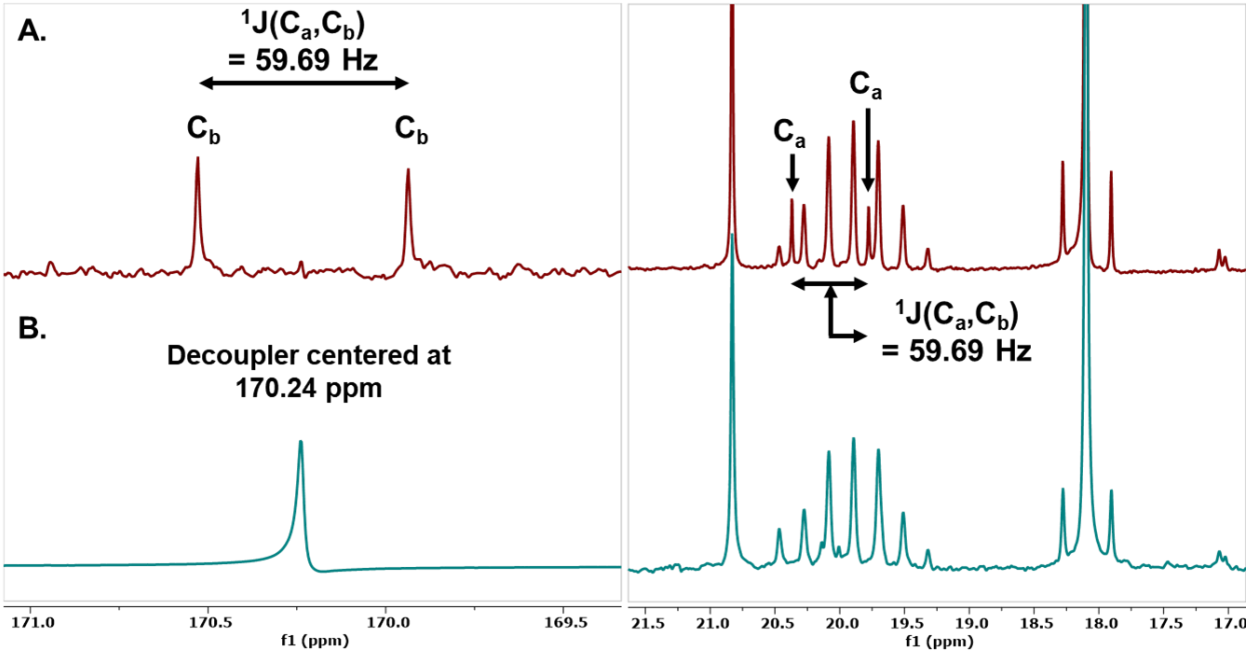
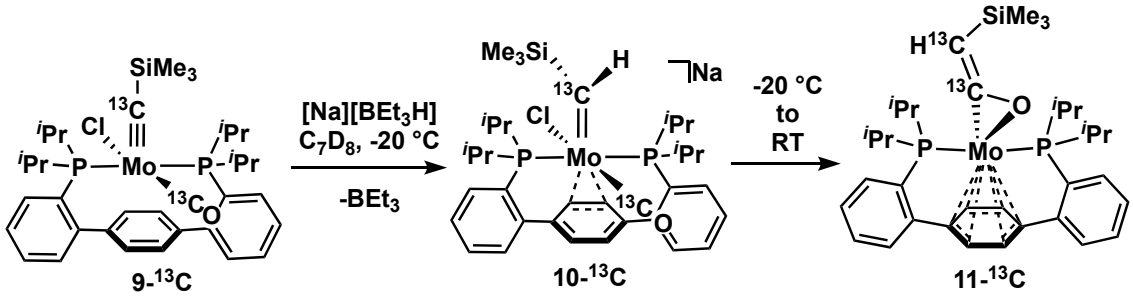


Figure S30—Partial $^{13}C\{^1H\}$ NMR spectra (101 MHz, C_7D_8, 23 °C) of EtOAc-$^{13}C_2$, **10**, without (A) and with (B) selective ^{13}C decoupling.

Hydride addition of Silylcarbyne 9

*Addition of $NaBEt_3H$ to **9**—In Situ Formation of **10** & **11***



In a typical experiment, a J. Young NMR tube was charged with a maroon solution of **9**-^{13}**C** (25 mg, 0.035 mmol) in C_7D_8 in an inert atmosphere glovebox. The tube was sealed, removed from the box, and attached to a high vacuum manifold. The reaction was cooled to -78 °C by placing the J. Young tube in a dry ice/acetone bath and with a heavy Ar counterflow, a solution of $NaBEt_3H$ in PhMe (1.0 M, 0.036 mL, 0.036 mmol) was added via gastight microsyringe. No significant color change was observed. The sample was sealed and carefully transferred to an NMR spectrometer, pre-cooled to -40 °C.

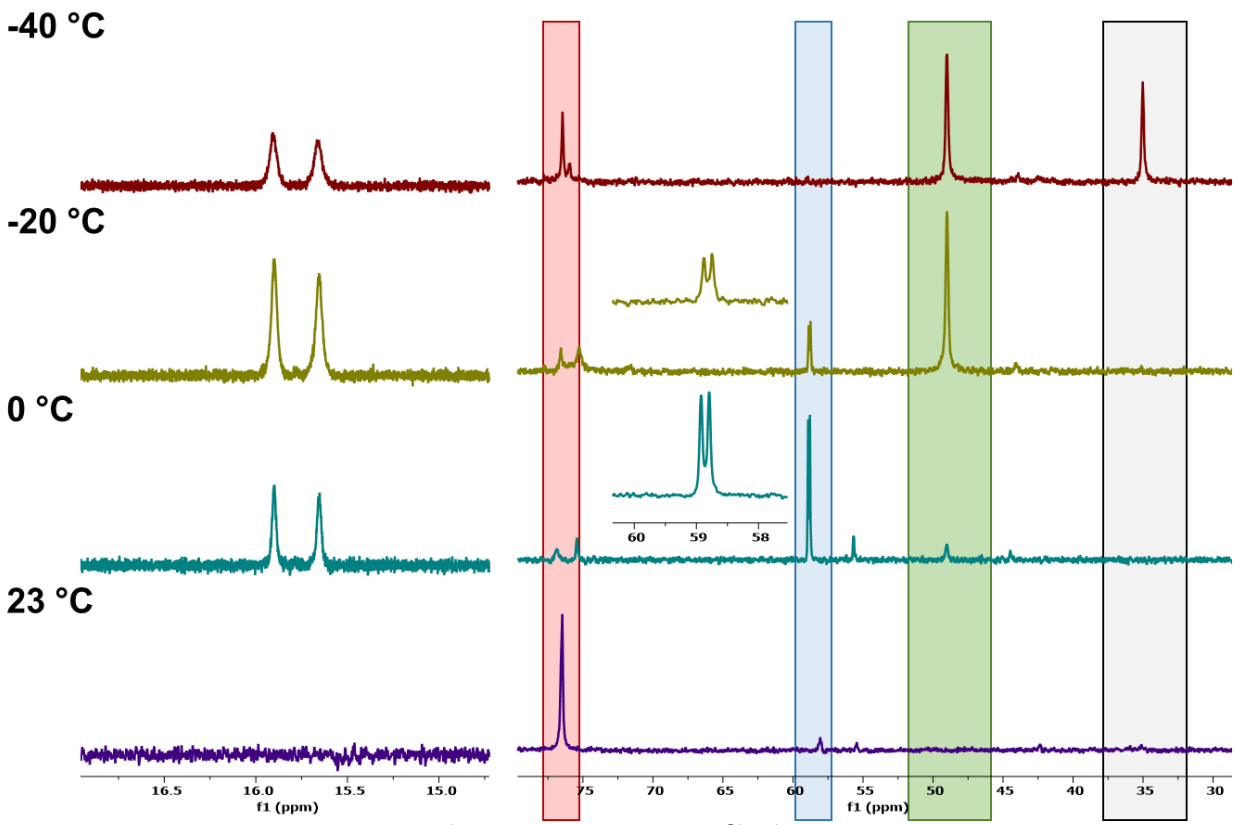


Figure S31—Variable temperature partial ^{1}H (500 MHz, C_7D_8) and ^{31}P{^{1}H} (202 MHz, C_7D_8) NMR spectra monitoring the addition of $NaBEt_3H$ to silylalkylidyne **9-^{13}C** (grey). At -40 °C, conversion to silyl carbene **10-^{13}C** (green) is observed. Further warming to -20 °C demonstrates conversion of **10-^{13}C** to ketene complex **11-^{13}C** (blue). Standing for 12 hr at room temperature results in clean conversion to Mo(0)-N_2 adduct **12** (red).

Following introduction of the sample, the probe was re-tuned to the appropriate nuclei and the sample locked and shimmed. During this time (*ca.* 15 minutes), slow conversion of **9-^{13}C** to **10-^{13}C** proceeded. Silylalkylidene **10-^{13}C** is demarcated by a highly deshielded doublet in the ^{1}H NMR spectrum centered at 15.77 ppm (Fig. S24, left). This signal corresponds to a singlet in the ^{31}P{^{1}H} spectrum at 48.99 ppm (Fig. S24, right) and resonances in the ^{13}C{^{1}H} spectrum at 321.17 and 257.83 ppm for the alkylidene and carbonyl carbons, respectively (Fig S25).

While the ^{1}H and ^{13}C chemical shifts do not rule out a formyl complex, 2-D ^{1}H/^{13}C NMR spectra at -30 °C (Fig. S26) further support the proposed alkylidene structure of complex **10-^{13}C**. A strong HSQC cross-peak (Fig. S26, left) and a large scalar coupling in the ^{1}H-coupled ^{13}C NMR spectrum (^{1}J(C,H) = 121.7 Hz, Fig. S24), are consistent with the downfield proton (d, 15.77 ppm, ^{1}J(C,H) = 121.7 Hz) being bound to the carbon resonating at 314.68 ppm. A gHMBC experiment displays a three-bond coupling between this same carbon and the trimethylsilyl protons at 0.17 ppm (Fig. S26, right). Taken together, these data support a silyl alkylidene and rule-out an alkylidyne/formyl assignment.

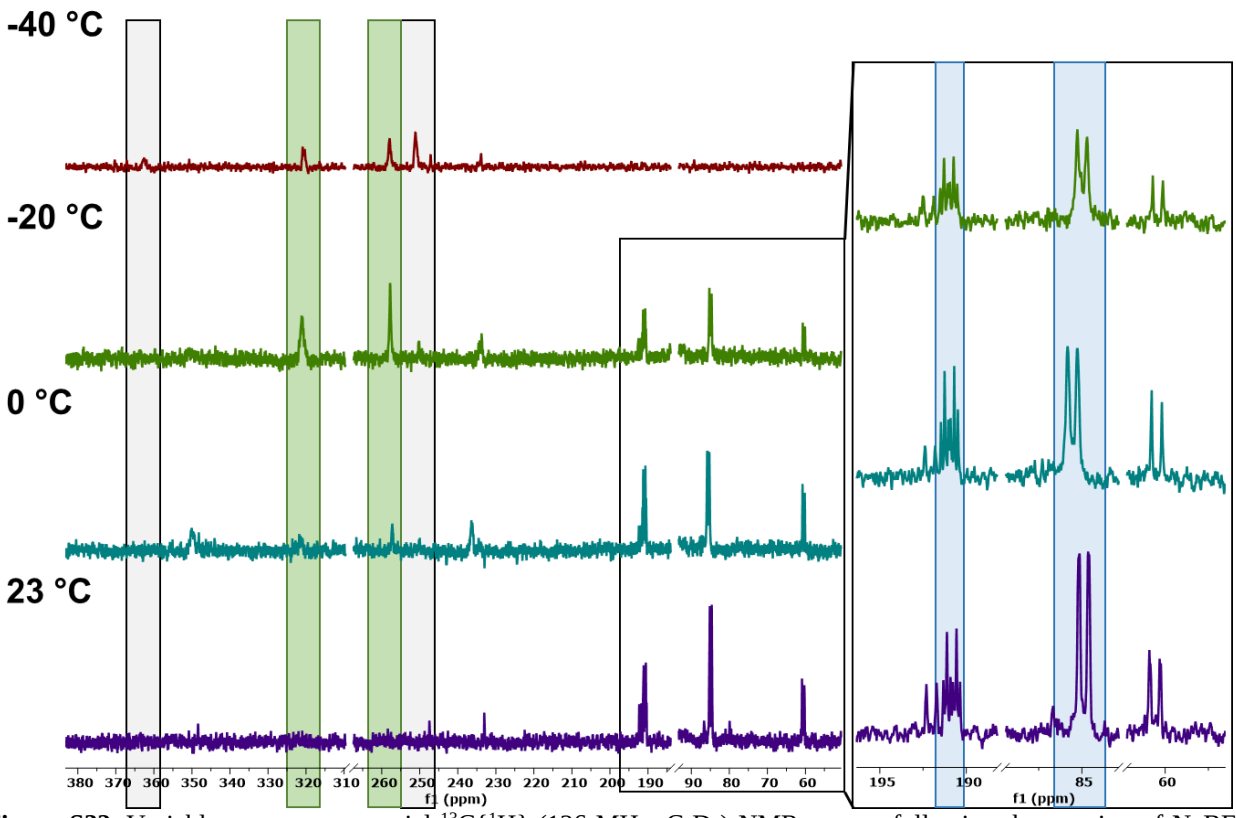


Figure S32. Variable temperature partial $^{13}C\{^{1}H\}$ (126 MHz, C_7D_8) NMR spectra following the reaction of $NaBEt_3H$ with silylalkylidyne **10-^{13}C** (grey). Upon warming, **10-^{13}C** is converted first to **11-^{13}C** (green), before C–C coupling affords ketene complex **12-^{13}C** (blue). Immediately upon warming to 23 °C, **12-^{13}C** is the major diamagnetic species present in solution, though free ketene-borane adduct, from ketene displacement by N_2, can also be detected (doublets at 192.10 and 60.59 ppm, ^{1}J(C,C) = 74.6 Hz). The inset shows an enlargement of the ketene resonances.

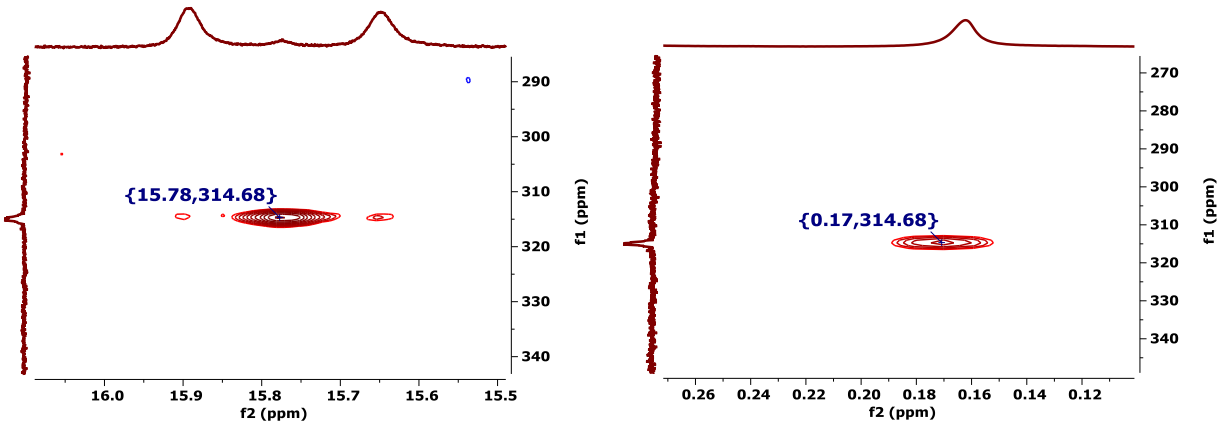


Figure S33—Partial $^{1}H/^{13}C$ HSQCAD (left) and HMBC (right) spectra (500/126 MHz, C_7D_8) of silylcarbene **10-^{13}C** at low temperature (-30 °C).

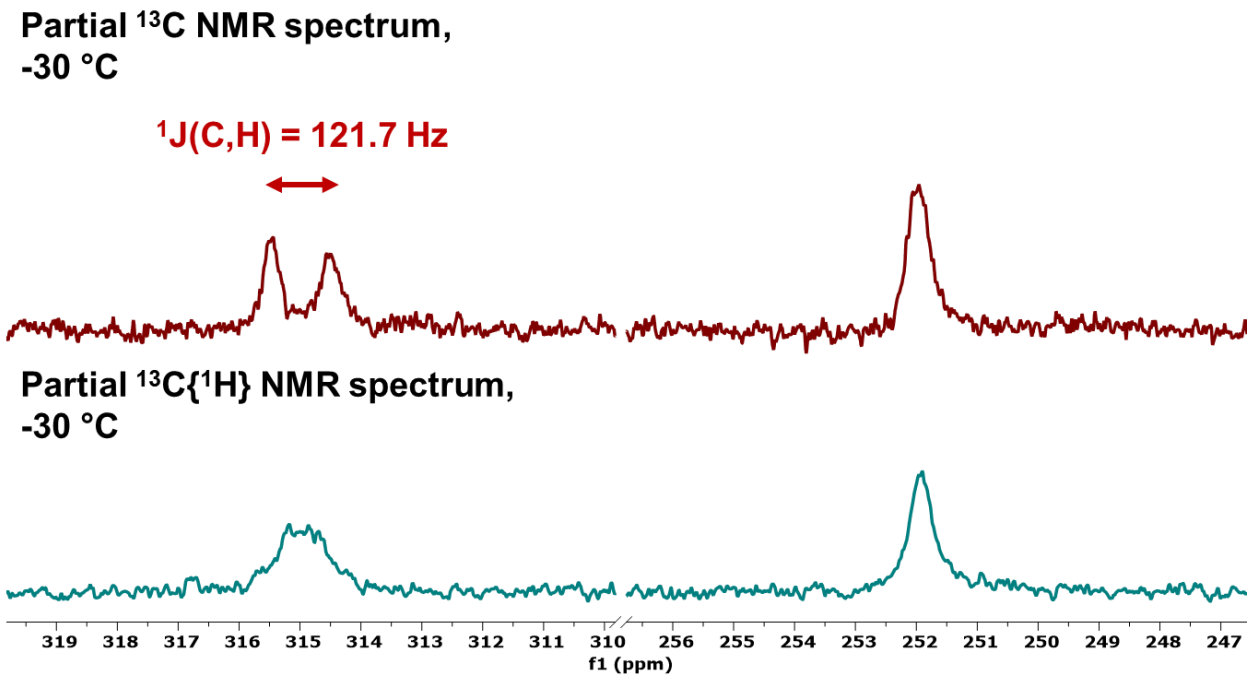


Figure S34—Partial low-temperature ^{13}C (126 MHz, C_7D_8, top) and $^{13}C\{^1H\}$ (126 MHz, C_7D_8, bottom) spectra of complex **10-^{13}C** . The ^1J(C,H) coupling constant extracted from the proton coupled spectrum shows good agreement with the ^1J(C,H) assigned to the downfield doublet in the ^1H NMR spectrum (15.77 ppm, J = 127.7 Hz).

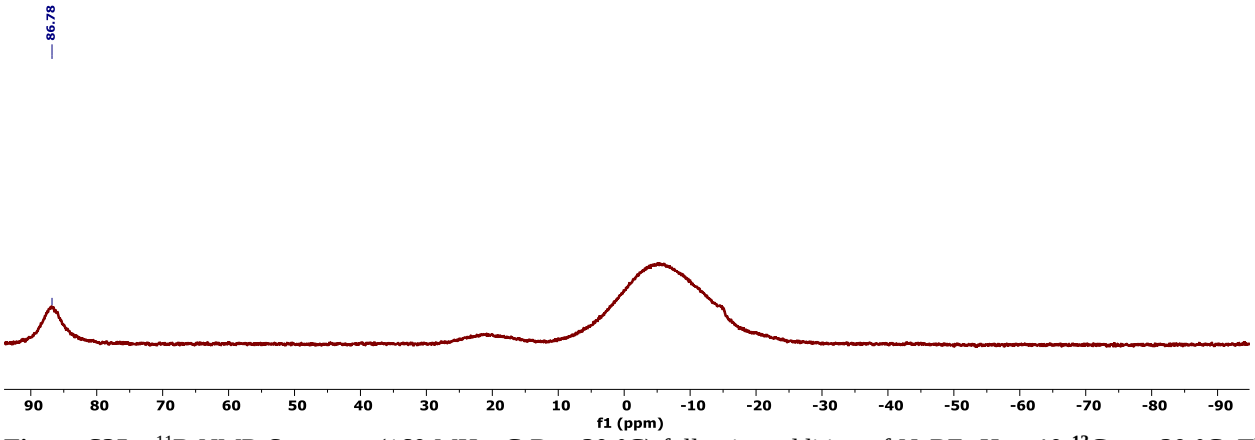


Figure S35—^{11}B NMR Spectrum (160 MHz, C_7D_8, -30 °C) following addition of $NaBEt_3H$ to **10-^{13}C** at -30 °C. The broad signal at 86.78 ppm is consistent with free BEt_3,[12] liberated after hydride transfer to **10-^{13}C** . The broad signal from -25 to 10 ppm corresponds to a borosilicate glass background.

Warming the sample in the NMR probe from -40 to -20 °C showed complete consumption of starting material by $^{31}P\{^1H\}$ NMR spectroscopy and the onset of formation of trimethylsilylketene complex **11-^{13}C** (d, 58.86 ppm, ^2J(P,C) = 25.49 Hz, Fig. S6). With further warming, substantial conversion to **11-^{13}C** is observed. A distinctive doublet of triplets (190.87 ppm, ^1J(C,C) = 70.26 Hz & ^2J(P,C) = 25.29 Hz) and doublet (85.52 ppm, ^1J(C,C) = 70.14 Hz) in the $^{13}C\{^1H\}$ NMR spectrum are consistent with a η^2-C,O ketene binding motif. Concomitant with these features, a pair of doublets (192.03 & 60.47 ppm, ^1J(C,C) = 72.83 Hz) grew in with increased temperature, assigned to a ketene-borane adduct. After sitting at room temperature for 12 h, Mo-N_2 complex **12** was the primary diamagnetic product ($^{31}P\{^1H\}$ NMR, Fig. S6 bottom).

A ketene/N_2 binding equilibrium was supported by addition of independently synthesized trimethylsilylketene to authentic **12** (Fig. S11). Addition of a single equiv. of ketene (0.021 mL, 0.5 M in C_6D_6) to a solution of **12** in C_6D_6 (25 mg, 0.042 mmol, in 0.5 mL) in a J. Young NMR tube under N_2 yields a mixture of **11** and **12**. A similar addition of five equiv. (0.105 mL, 0.5 M in C_6D_6) results in complete conversion to the ketene complex **11**.

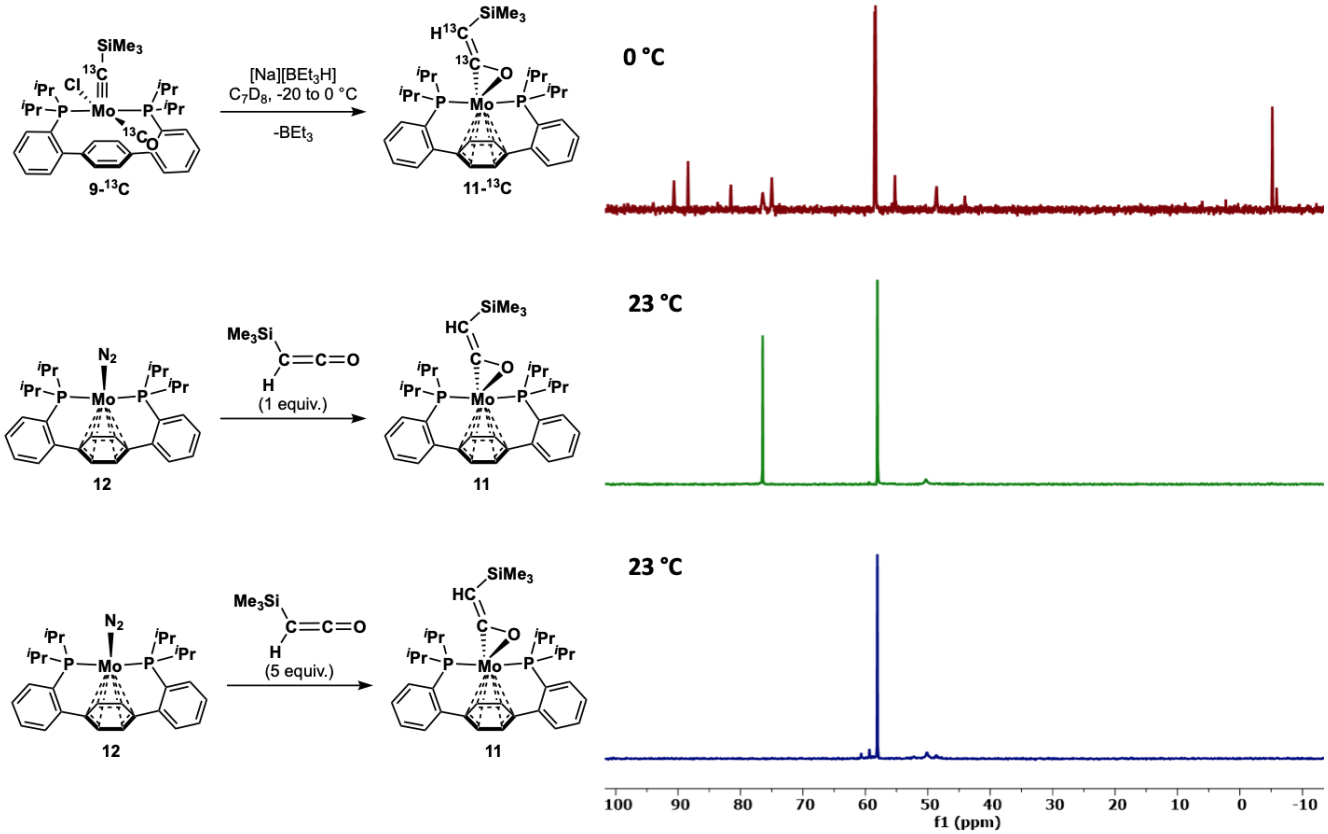


Figure S36—$^{31}P\{^1H\}$ NMR spectra showing the independent synthesis of trimethylsilylketene complex **11** via addition of authentic trimethylsilylketene to N_2 adduct **12** (middle & bottom). Note: The spectrum of **11-^{13}C** is included (top) for comparison. ^{13}C labeling in the top reaction affords a doublet (^2J(P,C) = 26.6 Hz), while the unlabeled trimethylsilylketene in the middle and bottom reactions gives a singlet; however, the chemical shift corroborates the proposed assignment.

*Crystallization of trimethylsilylketene complex **11***

Single crystals of complex **11** were obtained via slow evaporation of liquid butane, as follows:

A small swivel frit was assembled with a 50 mL round-bottom flask charged with **9** (50 mg, 0.070 mmol) and a small a stir bar at one end and a 50 mL round-bottom flask charged with a stir bar at the other. The apparatus was sealed, and evacuated. PhMe (*ca.* 7 mL) was admitted to the flask containing **9** at -78 °C via vacuum transfer, resulting in a deep red solution. With a heavy argon counterflow, the Teflon pin in the side arm of the swivel frit was replaced with a rubber septum. The septum was pierced with a 12-gauge needle and an 8" section of Teflon cannula was carefully inserted. A $NaBEt_3H$ solution in PhMe (0.5 M, 0.14 mL, 0.070 mmol) was introduced to the stirring reaction mixture via syringe through the short cannula. PhMe (0.20 mL) was injected through the same canula as a rinse. The Teflon pin was replaced, sealed, and the reaction placed in an ice water bath (0 °C) and left to stir for 2 hours. Volatiles were removed *in vacuo*, maintaining a temperature between 0 and 10 °C.

The residue remaining in the flask was extracted with butane (*ca.* 30 mL, freeze-pump-thawed x 3 and condensed from a -78 °C trap), introduced via vacuum transfer at -196 °C. A spatula wrapped with pipe cleaner was used to brush a -78 °C dry ice/acetone slurry onto the sidewalls of the swivel frit. It is imperative to keep the entire

apparatus cold during the filtration step. The top of the swivel frit (empty 50 mL flask) was then pre-cooled with liquid nitrogen and the frit swiveled, utilizing a -78/-196 °C temperature gradient to draw the butane filtrate through the frit.

The side-arm pin was once more replaced with a septum which was pierced with a 21-gauge needle. Solvent was evaporated at low temperature (-10 to 0 °C), with the aid of a slow argon flow, providing orange single crystals of **11**.

Thermochemical Studies.

Synthesis of $NaBHPh_3$

$NaBHPh_3$ was prepared according to the reported procedure,[13] only in THF instead of Et_2O to allow heating to higher temperatures. Thus, solid NaH (25.4 mg) was added to a solution of BPh_3 (256 mg, 1.06 mmol) in THF (2 mL). The reaction was heated (50 °C) for 16 h, filtered, and the filtrate concentrated in vacuo. The resulting sticky residue was lyophilized from benzene to remove residual THF. ^{1}H NMR analysis revealed complete consumption of BPh_3, and formation of a new species, with a key hydridic quartet (1:1:1:1 intensity, consistent with splitting by the ^{11}B nucleus) visible at 2.87 ppm. Integration of the ^{1}H NMR spectrum revealed the retention of 1.5 equiv THF that could not be removed on further drying. ^{1}H NMR (400 MHz, C_6D_6, 23 °C): 7.48 – 7.42 (m, 6H, Ph*H*), 7.18 – 7.11 (m, 6H, Ph*H*), 7.03 – 6.97 (t, J = 7.3 Hz, 3H, Ph*H*), 2.78 (1:1:1:1 q, J = 73.2 Hz, B*H*). ^{11}B NMR (128 MHz, C_6D_6, 23 °C): -7.81 (app s).

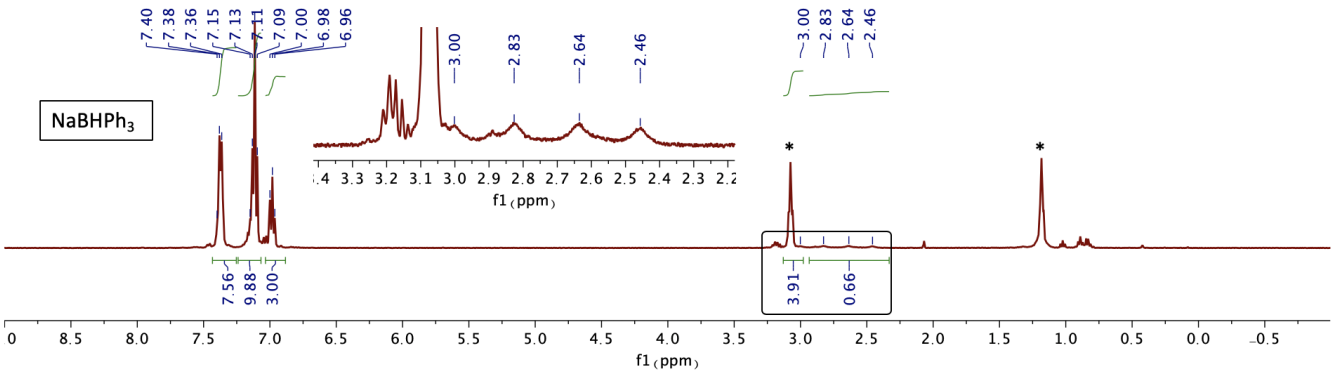


Figure S37—^{1}H NMR spectrum (400 MHz, C_6D_6, 23 °C) of $NaBHPh_3$. The inset shows a magnification of the key hydridic quartet.

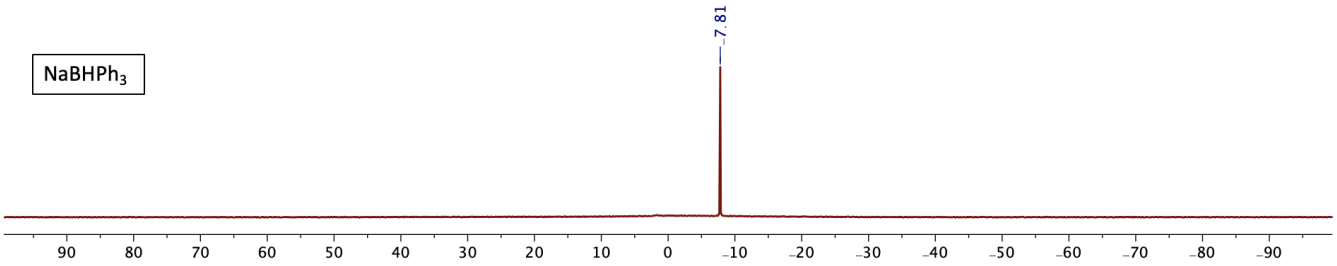
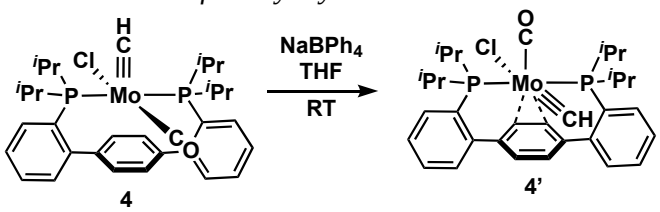


Figure S38—^{11}B NMR spectrum (128 MHz, C_6D_6, 23 °C) of $NaBHPh_3$.

*Independent Synthesis and Characterization of Methylidyne **4'***



To a suspension of **4** (50.0 mg, 0.079 mmol) in THF (3 mL) was added $NaBPh_4$ (26.9 mg, 0.079mmol, 1 equiv) in THF (1 mL). The reaction was stirred for 3 h at RT, during which time all solid **4** dissolved. No color change was apparent during this time. The reaction was concentrated in vacuo to dryness, and suspended in benzene (5 mL). Filtration resulted in recovery of a white solid whose ^{1}H and ^{11}B NMR shifts matched those of an authentic sample of $NaBPh_4$ (^{1}H NMR (400 MHz, THF, 23 °C): 7.32 – 7.24 (br m, 8H), 6.86 (t, *J* = 7.4 Hz, 8H), 6.71 (t, *J* = 7.1 Hz, 4H). ^{11}B NMR (MHz, THF, 23 °C): -8.65 ppm (s)). Lyophilization of the filtrate yield **4'** as an orange, free-flowing solid (35 mg, 70%). ^{1}H NMR (400 MHz, C_6D_6, 23 °C): 7.55 – 7.49 (m, 2H, aryl-*H*), 7.45 – 7.39 (m, 2H, aryl-*H*), 7.26 – 7.15 (m, 4H, aryl-*H*), 7.07 (s, 2H, aryl-*H*), 6.82 (tt, *J* = 4.3 Hz, *J* = 0.9 Hz, 2H, aryl-*H*), 2.83 – 2.68 (m, 2H, C*H*(CH_3)$_2$), 2.64 (t, *J* = 3.8 Hz, Mo≡C*H*), 2.39 – 2.25 (m, 2H, C*H*(CH_3)$_2$), 2.01 – 1.91 (m, 6H, CH(C*H*$_3$)$_2$), 1.63 – 1.55 (m, 6H, CH(C*H*$_3$)$_2$), 0.99 – 0.91 (m, 6H, CH(C*H*$_3$)$_2$), 0.77 – 0.70 (m, 6H, CH(C*H*$_3$)$_2$). $^{13}C\{^{1}H\}$ NMR (101 MHz, C_6D_6, 23 °C): 267.76 (t, $^{3}J_{CP}$ = 18.3 Hz, Mo≡*C*H), 241.19 (t, $^{3}J_{CP}$ = 11.2 Hz, *C*O), 148.67 (t, *J* = 6.4 Hz, aryl-*C*), 142.52 (t, *J* = 2.2 Hz, aryl-*C*), 132.03 (s, aryl-*C*), 130.70 (t, *J* = 10.5 Hz, aryl-*C*), 129.79 (s, aryl-*C*), 129.29 (t, *J* = 2.3 Hz, aryl-*C*), 128.17 (s, aryl-*C*), 127.93 (s, aryl-*C*), 101.87 (s, aryl-*C*), 35.38 (*t*, *J* = 10.1 Hz, *C*H(CH_3)$_2$), 30.83 (t, *J* = 8.0 Hz, *C*H(CH_3)$_2$), 20.03 (overlapping s, CH(*C*H$_3$)$_2$), 20.00 (overlapping s, CH(*C*H$_3$)$_2$), 19.79 (t, *J* = 4.1 Hz, CH(*C*H$_3$)$_2$), 18.56 (s, CH(*C*H$_3$)$_2$). $^{31}P\{^{1}H\}$ NMR (162 MHz, C_6D_6, 23 °C) δ: 41.81. FTIR (ATR, cm^{-1}): 1929 (C≡O). Vapor diffusion of pentane into THF solutions of **4'** yielded large, single crystalline blocks that needed to be cut for X-ray crystallographic analysis. A single-crystal XRD structure of **4'** corroborates the assignment of **4'** as the isomer drawn above (see Figure S50 below).

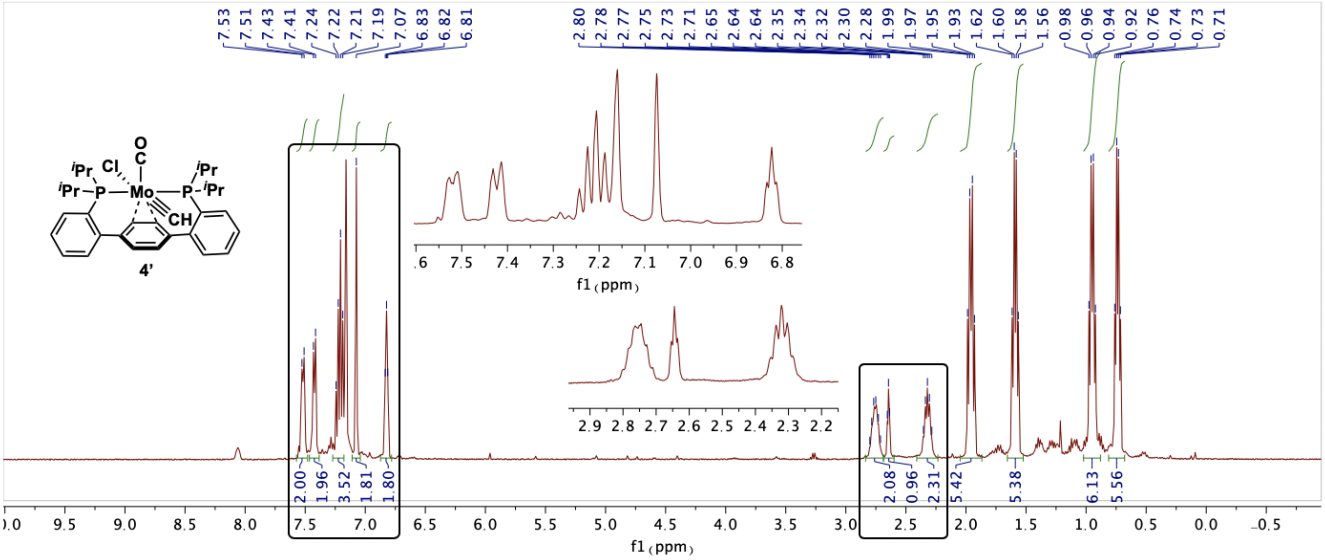


Figure S39—^{1}H NMR spectrum (400 MHz, C_6D_6, 23 °C) of **4'**.

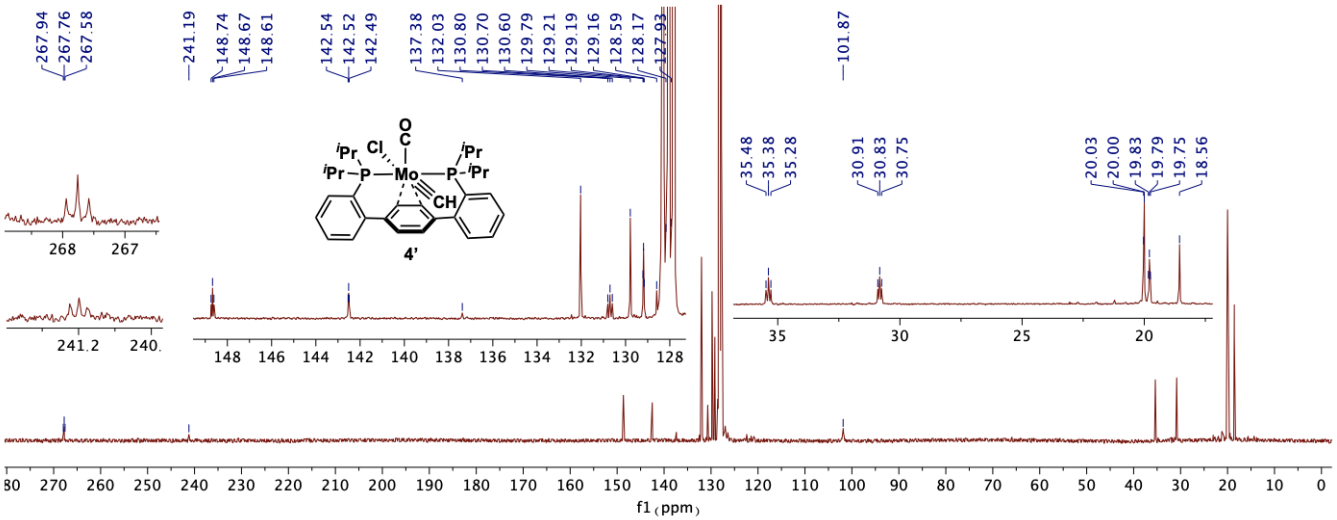


Figure S40—$^{13}C\{^{1}H\}$ NMR spectrum (MHz, C_6D_6, 23 °C) of **4'**.

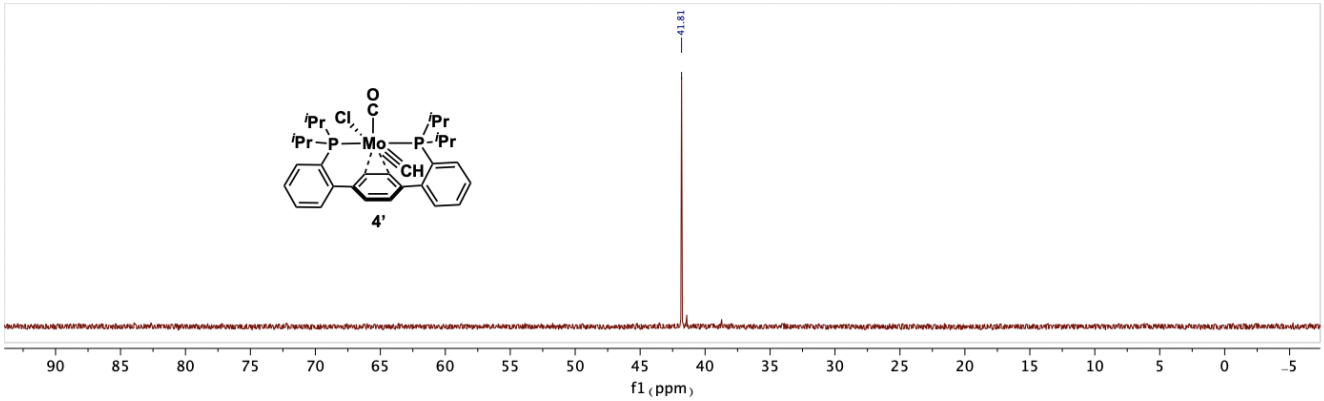


Figure S41—$^{31}P\{^{1}H\}$ NMR spectrum (400 MHz, C_6D_6, 23 °C) of **4'**.

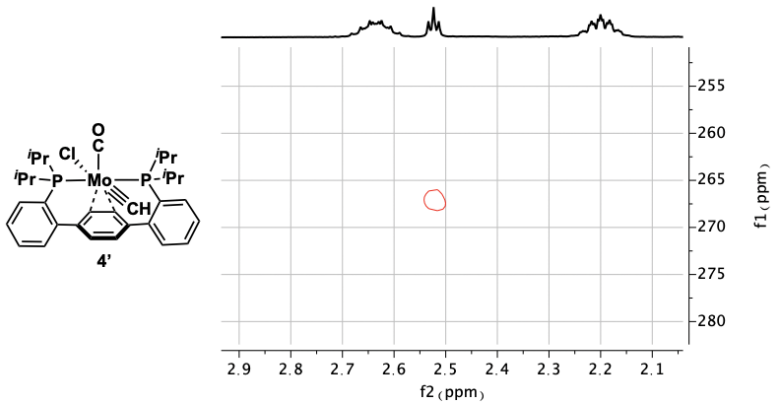
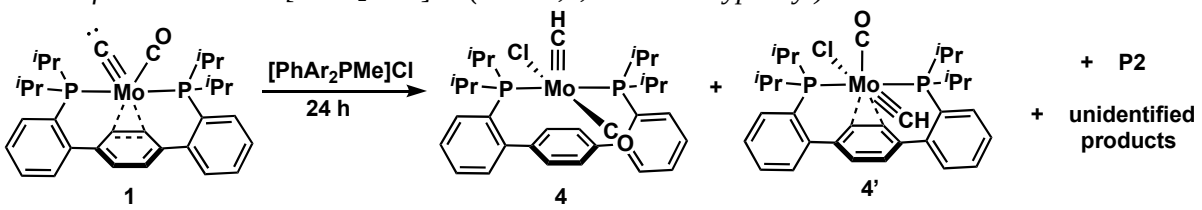


Figure S42—Partial $^{1}H/^{13}C$ HMQC spectrum (MHz, C_6D_6, 23 °C) showing that the key ^{1}H resonance at 2.64 ppm assigned to the methylidyne proton in **4'** correlates to the diagnostic ^{13}C triplet at 267.8 ppm in the corresponding $^{13}C\{^{1}H\}$ NMR spectrum.

*Protonation of carbide **1** with [PhAr$_2$PMe]Cl (Ar = 2,4,6-trimethoxyphenyl)*



In the glovebox, a thawing dark red solution of carbide **1** (0.047 mmol), prepared as above, was added to a thawing, stirring suspension of [PhAr$_2$PMe]Cl (23.3 mg, 0.047 mmol, 1 equiv) in THF. The reaction was stirred for 24 h, during which time the solid [PhAr$_2$PMe]Cl dissolved, and the color of the solution changed to dark brown. NMR analysis at this point confirmed complete consumption of the carbide, and formation of methylidyne **4**, its isomer **4'**, free **P2**, and several unidentified products. The expected conjugate base H$_2$C=CHPAr$_2$Ph (δ_P 162 MHz, THF, 23 °C: 7.00) was not observed, possibly reflecting its reactivity with **4** and/or **1**. ^{31}P{^{1}H} NMR (162 MHz, THF, 23 °C): 82.52 (s, 3%; unidentified), 72.26 (3 s, 7%; unidentified), 41.86 (s, 28%; **4'**), 41.41 (s, 8%; **4**), 7.90 (s, 10; unidentified), -1.57 (s, 4%; unidentified), -3.35 (s, 27%; **P2**), -4.41 (br s, 13%; unidentified).

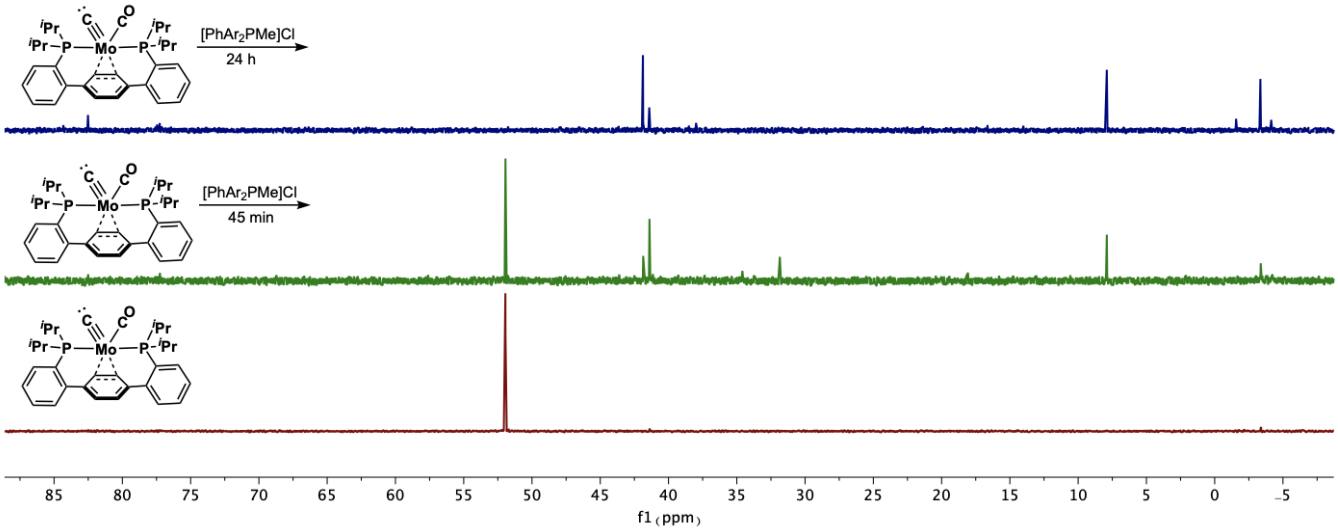
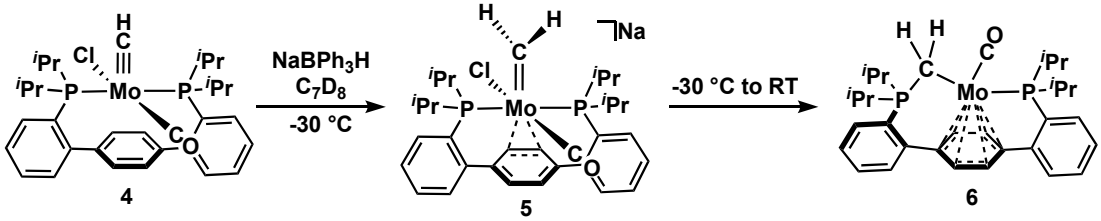


Figure S43—^{31}P{^{1}H} NMR spectra (162 MHz, C$_6$D$_6$, 23 °C) showing protonation of carbide **1** with [PhAr$_2$PMe]Cl (Ar = 2,4,6-trimethoxyphenyl). Bottom: carbide **1** prepared in situ via deprotonation of methylidene **4**. Middle: After addition of [PhAr$_2$PMe]Cl, *t* = 45 min; at this point, solid [PhAr$_2$PMe]Cl remains in suspension. Top: *t* = 24 h.

*Reaction of methylidyne **4** with NaBHPh$_3$: variable-temperature NMR study*



In the glovebox, a thawing solution of NaBHPh$_3$ (17.7 mg, 0.047 mmol in 0.5 mL THF), frozen in a glovebox cold well chilled with LN$_2$, was added dropwise to a thawing suspension of methylidyne **4** (30.0 mg, 0.047 mmol) in 2.0 mL THF. The suspension was re-frozen and, on thawing, transferred to a pre-chilled NMR tube. The NMR tube was re-frozen, and then transferred to a –78 °C cold bath outside of the glovebox. Insertion into an NMR probe pre-chilled to –50 °C showed persistence of **4**, with no apparent conversion to either methylidene **5** or ylide complex **6**. The tube was warmed incrementally in the spectrometer probe, showing the growth of ca. 40% **5**, and ca. 20% **6**, at

–30 °C over 1 h. Starting **4**, and its isomer **4'**, account for the balance. $^{31}P\{^{1}H\}$ NMR (162 MHz, C_7H_8, –30 °C): 41.01 (s, 24%; **4**), 41.50 (s, 16%; **4'•Cl**), 48.09 (d, $^{2}J_{PP}$ = 17.1 Hz, %; Mo*P* of **6**), 49.39 (s, 40%; **5**) 85.13 (d, $^{2}J_{PP}$ = 17.1 Hz; *P*CH_2 of **6**). Warming to –20 °C resulted in near-complete consumption of **4** over 1 h, with conversion to **4'•Cl**, **5** and ultimately **6**. After 1 h at –20 °C: $^{31}P\{^{1}H\}$ NMR (162 MHz, C_7H_8, –30 °C): 2% **4**, 16% **4'•Cl**, 75% **6**, 7% **5**. At 25 °C, remaining **4'Cl** and **5** were immediately consumed, and **6** was observed as the sole ^{31}P-containing product. $^{31}P\{^{1}H\}$ NMR (162 MHz, C_7H_8, –30 °C): 100% **6**.

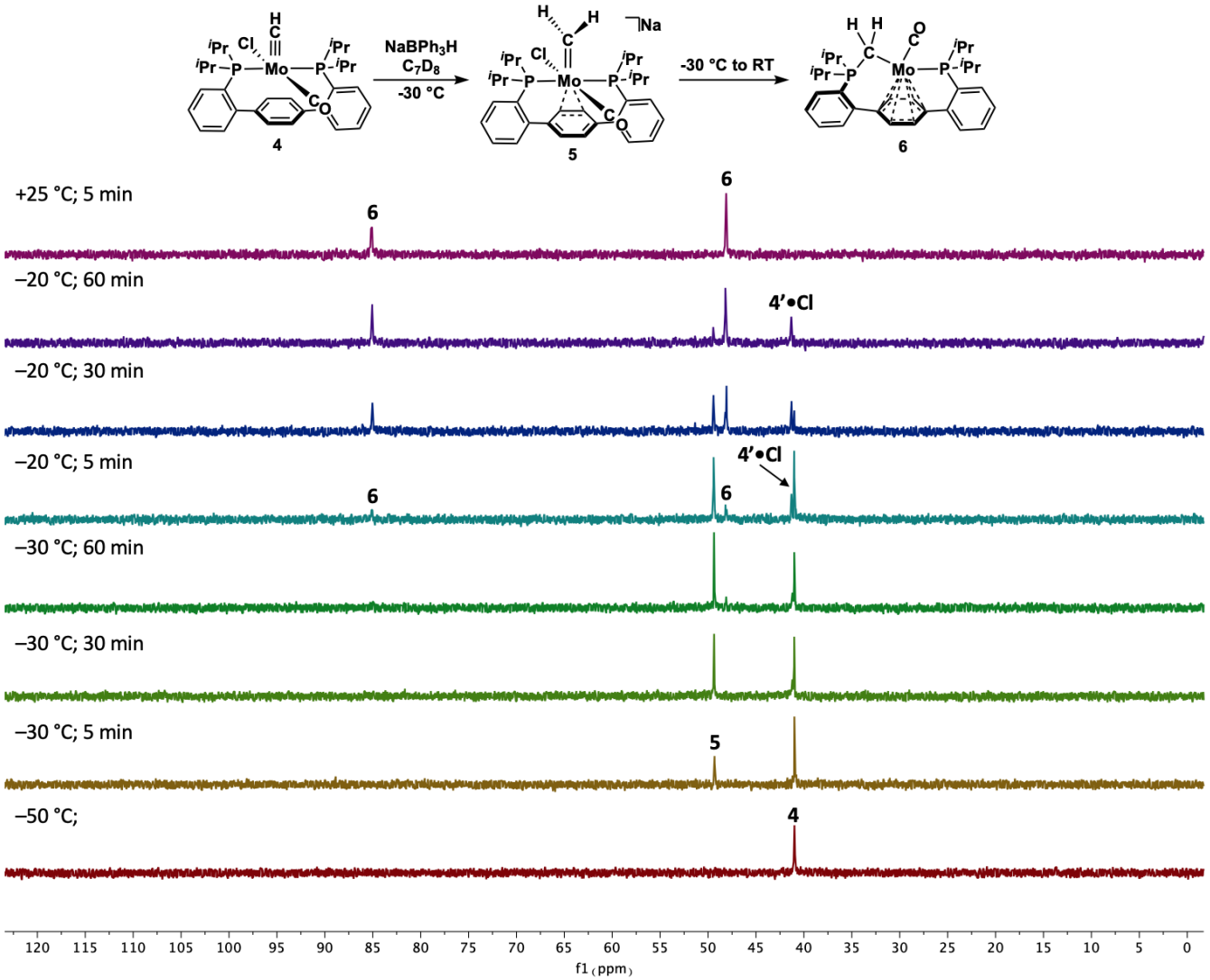


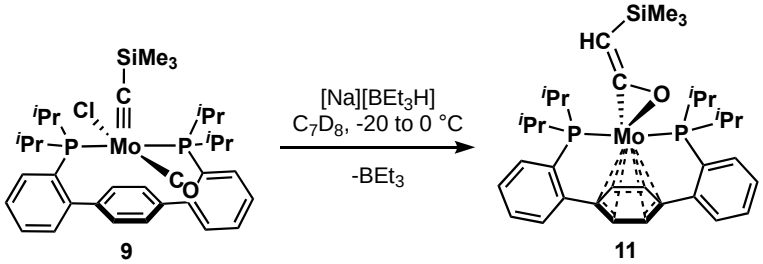
Figure S44—Variable-temperature $^{31}P\{^{1}H\}$ NMR spectra (162 MHz, C_6D_6) showing low-temperature conversion of methylidyne **4** to methylidene **5** and ylide complex **6** on addition of $NaBHPh_3$.

COMPUTATIONAL DETAILS

General Considerations

All quantum mechanics (QM) computations were performed using the M06-2X functional[14] of density functional theory (DFT) with the LACVP basis set[15] (based on 6-311g with an ECP for Mo), the LACV3P*+ extended basis set (a triple-zeta contraction of the LACVP basis set developed by Schrodinger) (including diffuse (+) and polarization (*) functions for all elements except Mo and H), and the 3-21g basis set[16-18] implemented in the Schrodinger Jaguar Software.[19]

Proposed Reaction Mechanism



In order to find a plausible reaction pathway between the silylalkylidyne complex **9** and the ketene complex **11**, a relaxed reaction coordinate scan using the C–C bond distance as the reaction coordinate was performed. At each point, the C–C bond distance is fixed and the rest of the molecule is relaxed. With a large molecule (*ca.* 100 atoms) such as this, this relaxed coordinate scan proved more convenient than trying to find a transition state using such algorithms as the quadratic synchronous transit (QST) method. Additionally, the system was truncated by replacing the borane ethyl groups with methyl groups. All calculations were performed in the gas phase, which is a reasonable approximation of the toluene solvent (which has a dielectric constant between 2.6 and 2.4 over the reaction relevant temperature range of -78 to -20°C).[20] The solution state structure of the Mo complexes are also assumed to be monomeric, most consistent with experimental data.

As the C–C scan goes through distances of *ca.* 2.1A, the complex undergoes a singlet to triplet crossing (Fig. S25), at an energy 15 to 20 kcal/mol above the ground state, a reasonable barrier for the experimental reaction conditions (273 K). Throughout the reaction, the spin density of the triplet and spin-unrestricted singlet remains localized on the Mo center.

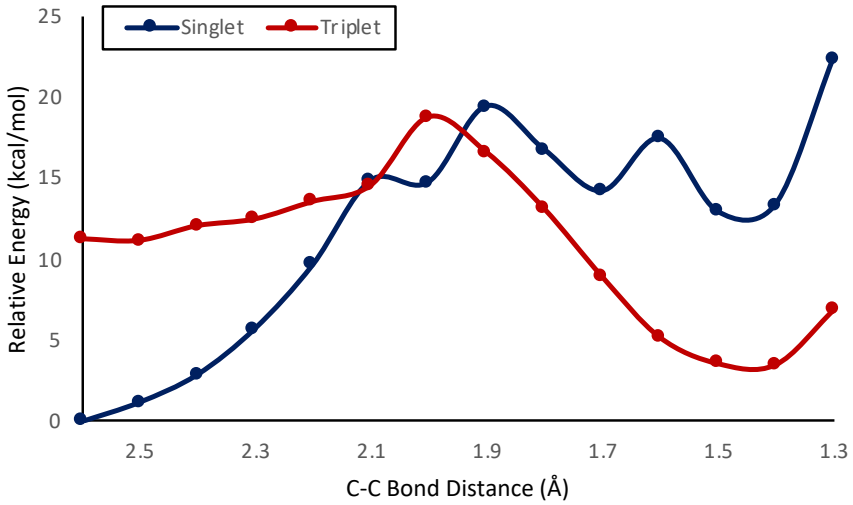


Figure S45—Potential energy landscape of C–C bond formation. Optimizations using M06-2X/LACV3P*+.

A coordinate system with that the z-axis along the Mo-alkylidyne vector, the y-axis along the P-Mo-P vector, and the x-axis along the Mo-CO vector was selected (Fig. S26, inset). The reaction proceeds as follows:

- As the C–C distance contracts from 2.6 to 2.1 Å, the alkylidene rotates 90° for both the singlet and the triplet.
- At the minimum energy crossing point between the singlet and triplet states (C–C *ca.* 2.1 Å), an electron is promoted from the doubly occupied HOMO (d_{yz} parentage; π-backbonding between the Mo and arene) to the LUMO+1 (d_{xz} parentage; π* between the Mo and alkylidene, Fig. S26). Occupation of this π* orbital corresponds to formal scission of the π-bond between the alkylidene and metal center. Phosphine dissociation can be ruled out; all such pathways gave proceeded with higher energy barriers than are reasonable given the experimental conditions.
- As the C–C distance decreases further, a Mo(C–C) metallocyclopropane begins to form.
- Near C–C = 1.4 Å, the ketene isomerizes from a η^2-C,C bound structure to an η^2-C,O bound structure. Based on the experimental crystal structure we know that the Na^+, Cl^-, and borane must dissociate in forming the final product, **11**, and the system must relax back to a singlet ground state. This dissociation/relaxation process was not investigated computationally as the dissociation of ionic species demands explicit solvent treatment.
- However, from the computed η^2-C,O intermediate, the η^2 metal–arene interaction must slip to an η^6 binding mode, affording the 18 valence electron species that was characterized in the solid-state.

We find that the borane, Na^+, and Cl^- are all required for a low energy pathway to ketene formation. Exclusion of any of these species results in an unrealistic reaction barrier, approximately 10 kcal/mol higher. The presence of Cl^- destabilizes the Mo d_{xy} and d_{xz} orbitals, the Na^+ acts as a Lewis acid to stabilize alkylidene activation (breaking the Mo=C($SiMe_3$)(H) double bond), and the borane polarizes the oxygen sp^2 lone pair, stabilizing CO double bond character and lowering the transition barrier between the ketene coordination isomers.

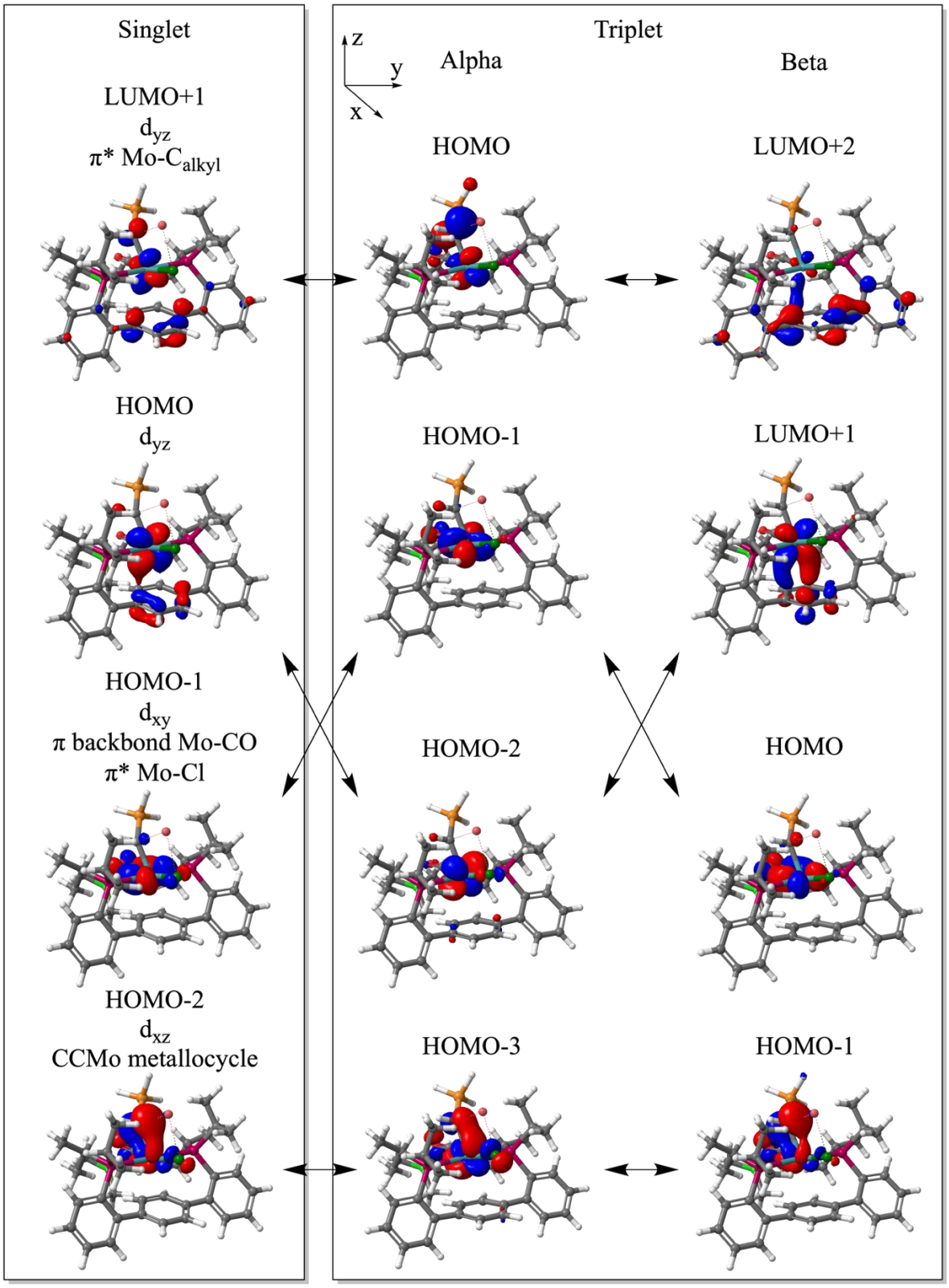


Figure S46—Frontier molecular orbitals near the minimum energy crossing point of C–C *ca.* 2.1 Å. The three highest occupied orbitals are largely metal-based, suggesting a d^6 electronic configuration, with significant metal-ligand covalency. The LUMOs for the singlet, alpha triplet, and beta triplet are all solely based on the Na^+.

A diagnostic coordinate to follow the changes in the electronic structure along the reaction pathway is the O–C–C–Si dihedral angle (Fig. S27). The alkylidene is most stable when the dihedral angle is near 0° (slight deviations result from the alkylidene-Na interactions). As the new C–C bond is formed, the dihedral angle jumps to 45° with a simultaneous increase in the C_{CO}–Mo–C_{alkyl}–Si dihedral angle from 0° to 90°. This alkylidene rotation is attributed to interactions between the π and π* orbitals on the ketene with the d-orbitals on the metal. Once the ketene isomerizes to the η^2-C,O structure, the O–C–C–Si dihedral angle returns to 0°, corresponding to the π and π* orbitals between the carbon and oxygen interacting with the metal. These π orbitals must be parallel to the substituents on the alkylidene carbon.

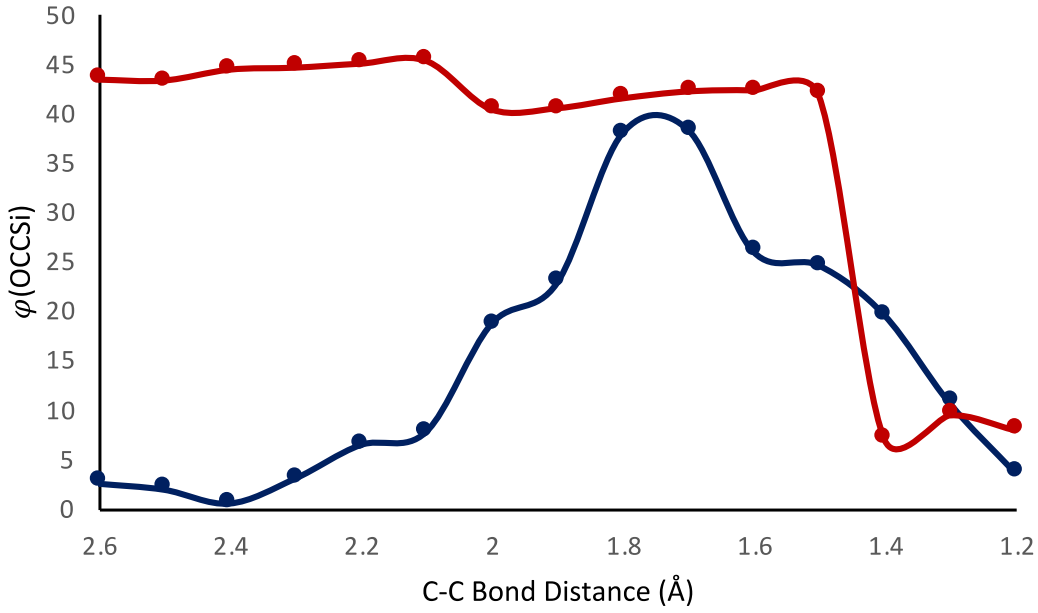


Figure S47—Ketene (O–C–C–Si) dihedral angle as a function of C–C distance. Optimization were conducted at a M06-2X/LACV3P*+ level of theory.

Additional Considerations

The following observations were made regarding the structures of intermediates to ketene formation:

- The alkylidene must be located *trans* to the arene (Fig. S28). Although the optimized *cis*-alkylidene structure is slightly more stable than the *trans*-alkylidene, the singlet-triplet crossing point occurs 10 kcal/mol lower for the *trans*-alkylidene. These energies suggest that the *trans*-species forms earlier in the reaction coordinate (likely directly from the *trans*-alkylidyne), and rearrangement between the isomers is energetically unfavorable.

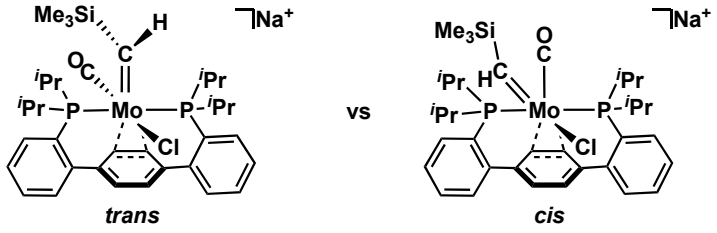


Figure S48—*trans*- (left) and *cis*-alkylidene (right) isomers considered in the DFT calculations.

- The structure with the silyl group of the alkylidene *"endo"* to the carbonyl is more stable than that with the silyl group *"exo"* by 2.25 kcal/mol (at the M06-2X/LACVP level of theory, Fig. S29). Notably, this structure maps onto with the XRD structure of silylketene **11**, following C–C bond formation and ketene-binding isomerization. The "*exo*" configuration (barring additional reorganization) would not afford the characterized structure.

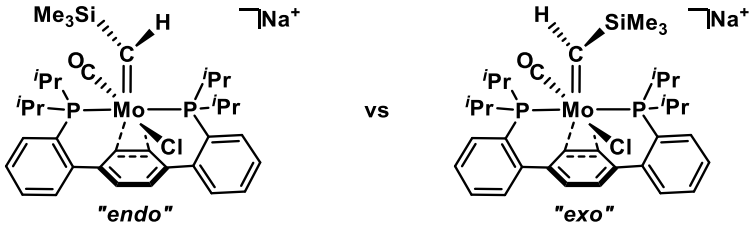


Figure S49—Optimized structures of the "endo" (left) and "exo" (right) $SiMe_3$/CO orientations of silylalkylidene **9**.

- Given experimental evidence for methylidene insertion into the Mo–P bond (from **5**), the same process from **10** was explored computationally. We are unable to find a stable structure with an inserted silylalkylidene. While this negative result does not prove that the insertion cannot occur, it is consistent with experiment, suggesting that this insertion is unfavorable.

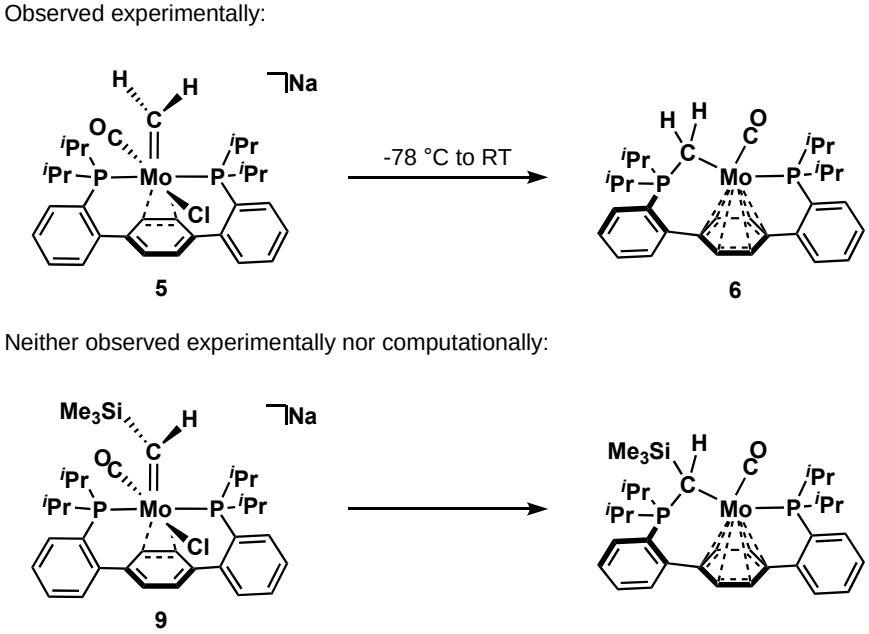


Figure S50—Parent methylidene and silylalkylidene insertions into Mo–P bonds.

Cartesian Coordinates of Molecules Along the Potential Energy Landscape (Figure S43)

Calculated Structure **1**: Singlet

Mo	0.11362	-0.60900	-0.23560
P	-2.54789	-0.44159	-0.48364
P	2.74691	-0.38785	-0.37060
O	0.08197	-1.57691	-3.09443
C	-1.35406	2.46392	0.23648
C	-0.61957	2.12068	-0.90309
C	0.76888	2.13369	-0.87203
C	1.44907	2.49768	0.29376
C	0.71464	2.94073	1.39097
C	-0.67344	2.92053	1.36318
C	-2.82913	2.33360	0.23208
C	-3.47703	1.14031	-0.14140
C	-4.87917	1.12653	-0.14230
C	-5.62505	2.23967	0.21700
C	-4.97631	3.40585	0.60738
C	-3.59197	3.44418	0.61360
C	2.92530	2.40202	0.34722
C	3.61860	1.22512	0.00101
C	5.01960	1.25988	0.04964
C	5.71722	2.39686	0.43223
C	5.02114	3.54222	0.79890
C	3.63697	3.53632	0.75432
C	-3.58545	-1.59235	0.57592
C	-3.20069	-3.05859	0.36668
C	-3.54091	-1.13001	2.04359
C	-3.05421	-0.91416	-2.22688
C	-2.65194	0.18197	-3.21744
C	-4.51512	-1.29707	-2.47133
C	3.76970	-1.52549	0.71028
C	3.47207	-1.27192	2.18695
C	3.63273	-3.00924	0.36229
C	3.31995	-0.83237	-2.09946
C	2.86871	0.21383	-3.12091
C	4.81295	-1.10770	-2.29668
C	0.08196	-1.13330	-1.99771
C	0.34444	-2.49552	0.20127
H	-1.13462	1.87986	-1.82359
H	1.32782	1.89722	-1.76806
H	1.22927	3.20422	2.30782
H	-1.23082	3.17299	2.25840
H	-5.41346	0.22420	-0.41049
H	-6.70790	2.19156	0.20053
H	-5.54621	4.28103	0.89754
H	-3.07481	4.35468	0.89644
H	5.59470	0.37906	-0.20187
H	6.80098	2.38142	0.45302
H	5.55262	4.43455	1.10919
H	3.08118	4.43029	1.01621
H	-4.61911	-1.50016	0.24144
H	-2.14134	-3.25709	0.54996
H	-3.36780	-3.37260	-0.66630
H	-3.80538	-3.70408	1.01035
H	-2.60620	-0.62480	2.31630
H	-3.72722	-1.96714	2.72745
H	-4.31680	-0.38878	2.23894
H	-2.42729	-1.79059	-2.42481
H	-3.16423	1.12244	-2.98917
H	-2.94482	-0.11422	-4.22778
H	-1.57594	0.34911	-3.23226
H	-4.90476	-2.03572	-1.76880
H	-4.59458	-1.73697	-3.46926
H	-5.16738	-0.42133	-2.45708
H	4.80905	-1.24797	0.52686
H	4.13136	-1.88735	2.80640
H	2.43770	-1.51723	2.42941
H	3.62523	-0.22582	2.46223
H	2.68894	-3.41752	0.71883
H	4.43716	-3.56341	0.85512
H	3.69732	-3.21285	-0.70786
H	2.75863	-1.75407	-2.29472
H	1.78619	0.32888	-3.14630
H	3.18095	-0.09607	-4.12180
H	3.33335	1.18403	-2.91585
H	5.38562	-0.17786	-2.30821
H	4.95865	-1.58264	-3.27090
H	5.24403	-1.77260	-1.54679
H	0.77723	-2.71419	1.20395
Si	0.32619	-3.98929	-0.90356
H	0.32730	-5.25468	-0.10375
H	-0.89887	-4.04030	-1.74512
H	1.49078	-4.08023	-1.82409
B	-0.43068	-2.72319	-5.20760
C	-0.16154	-1.40743	-6.03496
C	-1.91396	-3.13741	-4.85476
C	0.73091	-3.76925	-5.00308
H	0.88446	-1.09081	-6.03247
H	-0.43986	-1.59138	-7.08238
H	-0.77841	-0.56979	-5.69785
H	-1.98230	-3.63079	-3.88067
H	-2.63749	-2.31863	-4.89412
H	-2.23856	-3.88614	-5.59139
H	0.49354	-4.57604	-4.30551
H	0.96133	-4.23271	-5.97273
H	1.65352	-3.28553	-4.66923
Cl	0.11849	-0.03348	2.51865
Na	-1.00601	-2.24316	2.33758

Calculated Structure **2**: Singlet

Mo	0.06585	-0.61834	-0.19755
P	-2.59055	-0.44336	-0.39620
P	2.69835	-0.44733	-0.43452
O	-0.01724	-1.81893	-2.94705
C	-1.34703	2.47009	0.17637
C	-0.62970	2.08443	-0.96049
C	0.75904	2.08467	-0.94365
C	1.45698	2.46878	0.20449
C	0.73997	2.95060	1.29757
C	-0.64860	2.94943	1.28309
C	-2.82421	2.36530	0.18359
C	-3.49327	1.16997	-0.14144
C	-4.89524	1.18152	-0.14497
C	-5.62097	2.32219	0.16650
C	-4.95136	3.49083	0.51202
C	-3.56636	3.50402	0.51952
C	2.93223	2.34856	0.24137
C	3.60182	1.15597	-0.10141
C	5.00362	1.16903	-0.07674
C	5.72532	2.29928	0.28077
C	5.05349	3.45958	0.64545
C	3.66873	3.47566	0.62319
C	-3.62709	-1.49917	0.76038
C	-3.28900	-2.98652	0.63850
C	-3.52688	-0.94521	2.19223
C	-3.13063	-1.02845	-2.09458
C	-2.72704	-0.00781	-3.16222
C	-4.60087	-1.40387	-2.29534
C	3.73526	-1.60291	0.61206
C	3.49327	-1.34136	2.09746
C	3.54587	-3.08203	0.26972
C	3.20152	-0.91418	-2.18018
C	2.70812	0.11577	-3.19791
C	4.68666	-1.18752	-2.42914
C	-0.00186	-1.24878	-1.91000
C	0.24637	-2.50328	0.23816
H	-1.15783	1.81946	-1.86727
H	1.30536	1.81873	-1.83853
H	1.26706	3.22988	2.20263
H	-1.19397	3.23641	2.17545
H	-5.44542	0.27845	-0.37559
H	-6.70452	2.29363	0.14909
H	-5.50558	4.38716	0.76590
H	-3.03266	4.41546	0.76653
H	5.56031	0.27638	-0.32851
H	6.80890	2.26725	0.28330
H	5.60404	4.34703	0.93598
H	3.13195	4.38210	0.88209
H	-4.66760	-1.39805	0.44925
H	-2.22884	-3.20421	0.79294
H	-3.50497	-3.36672	-0.36222
H	-3.88253	-3.56945	1.34875
H	-2.55562	-0.48870	2.41934
H	-3.75556	-1.72103	2.93240
H	-4.24758	-0.14077	2.34570
H	-2.51898	-1.92670	-2.24017
H	-3.24368	0.94464	-3.00478
H	-3.01552	-0.38053	-4.14835
H	-1.65188	0.16444	-3.18574
H	-4.99867	-2.07318	-1.53065
H	-4.69830	-1.92179	-3.25346
H	-5.23663	-0.51785	-2.34946
H	4.77442	-1.35209	0.39238
H	4.15841	-1.97120	2.69577
H	2.46201	-1.56296	2.37395
H	3.67882	-0.29879	2.36605
H	2.59136	-3.45583	0.63538
H	4.33567	-3.66212	0.75615
H	3.59332	-3.28996	-0.80066
H	2.63626	-1.83991	-2.34464
H	1.62286	0.21496	-3.19143
H	2.99771	-0.19756	-4.20451
H	3.16470	1.09467	-3.01665
H	5.25854	-0.25729	-2.45681
H	4.79850	-1.66053	-3.40892
H	5.14229	-1.85462	-1.69582
H	0.70348	-2.72928	1.23136
Si	0.08841	-4.06398	-0.77120
H	0.01969	-5.24587	0.14485
H	-1.16430	-4.09998	-1.57029
H	1.21838	-4.32876	-1.70092
B	0.03096	-2.43446	-5.23050
C	-0.04660	-0.97881	-5.83921
C	-1.28862	-3.29087	-5.08647
C	1.43700	-3.14127	-5.09486
H	0.77078	-0.33085	-5.51194
H	0.05322	-1.06660	-6.93084
H	-0.99439	-0.46727	-5.65438
H	-1.19123	-4.11200	-4.37193
H	-2.15697	-2.68715	-4.80431
H	-1.52647	-3.74107	-6.06050
H	1.45099	-3.90267	-4.31112
H	1.66335	-3.65761	-6.03837
H	2.26012	-2.44277	-4.91611
Cl	0.19023	0.02003	2.54001
Na	-0.99325	-2.15951	2.44735

Calculated Structure **3**: Singlet

Mo	0.03210	-0.58288	-0.22642
P	-2.61793	-0.37628	-0.37454
P	2.66365	-0.42719	-0.50925
O	-0.09082	-1.84248	-2.93789
C	-1.33955	2.50541	0.25942
C	-0.63324	2.15021	-0.89436
C	0.75538	2.13695	-0.88435
C	1.46411	2.47224	0.27242
C	0.75827	2.92351	1.38573
C	-0.63017	2.93884	1.37807
C	-2.81766	2.42012	0.26861
C	-3.50149	1.24301	-0.08935
C	-4.90329	1.27231	-0.09121
C	-5.61409	2.41271	0.25397
C	-4.92955	3.56199	0.63354
C	-3.54453	3.55777	0.63931
C	2.93767	2.32981	0.29861
C	3.59004	1.14433	-0.09993
C	4.99194	1.13643	-0.07836
C	5.73025	2.23819	0.33024
C	5.07572	3.38997	0.74914
C	3.69141	3.42738	0.72974
C	-3.65212	-1.42491	0.79261
C	-3.35786	-2.91901	0.64853
C	-3.50078	-0.89265	2.22724
C	-3.18608	-0.94478	-2.06773
C	-2.76608	0.06621	-3.13823
C	-4.66476	-1.29082	-2.25934
C	3.69787	-1.66232	0.44385
C	3.48003	-1.49567	1.94659
C	3.47335	-3.11075	0.00625
C	3.13111	-0.80282	-2.28495
C	2.60245	0.26089	-3.24794
C	4.61266	-1.04863	-2.57527
C	-0.06041	-1.23028	-1.92518
C	0.16847	-2.48537	0.10764
H	-1.16964	1.92148	-1.80673
H	1.29379	1.89855	-1.79106
H	1.29265	3.16379	2.29761
H	-1.16817	3.20264	2.28201
H	-5.46507	0.38307	-0.34561
H	-6.69792	2.39833	0.23717
H	-5.47229	4.45705	0.91516
H	-2.99891	4.45454	0.91248
H	5.53545	0.24927	-0.37449
H	6.81321	2.19047	0.32910
H	5.63935	4.25499	1.07933
H	3.16848	4.32892	1.03054
H	-4.69730	-1.29197	0.50977
H	-2.30166	-3.16827	0.77914
H	-3.60499	-3.28439	-0.35037
H	-3.95101	-3.49265	1.36663
H	-2.50213	-0.49405	2.44349
H	-3.75963	-1.66300	2.96271
H	-4.17326	-0.05089	2.39959
H	-2.59374	-1.85517	-2.21522
H	-3.28184	1.02102	-2.99275
H	-3.04179	-0.31331	-4.12533
H	-1.69039	0.23664	-3.14698
H	-5.07417	-1.94275	-1.48563
H	-4.77844	-1.81605	-3.21156
H	-5.28119	-0.39181	-2.32023
H	4.73864	-1.41681	0.22633
H	4.14718	-2.16907	2.49283
H	2.45068	-1.72556	2.22300
H	3.67849	-0.47433	2.27959
H	2.50016	-3.47577	0.32827
H	4.23549	-3.74368	0.47025
H	3.53808	-3.25288	-1.07426
H	2.57267	-1.72626	-2.47668
H	1.51545	0.34202	-3.21210
H	2.87517	-0.00459	-4.27265
H	3.04905	1.23831	-3.03629
H	5.17741	-0.11360	-2.55750
H	4.71076	-1.46483	-3.58205
H	5.08490	-1.75341	-1.88913
H	0.64863	-2.76861	1.07831
Si	-0.11372	-4.04758	-0.88337
H	-0.26365	-5.18289	0.08185
H	-1.37445	-4.02532	-1.66867
H	0.98783	-4.43653	-1.80314
B	0.35775	-2.72525	-5.14772
C	-0.00307	-1.37244	-5.87665
C	-0.74561	-3.83903	-4.97411
C	1.87206	-3.08754	-4.87965
H	0.56622	-0.52527	-5.48367
H	0.27869	-1.46226	-6.93540
H	-1.06604	-1.12008	-5.84871
H	-0.46254	-4.64452	-4.29201
H	-1.69793	-3.41919	-4.63660
H	-0.94009	-4.29677	-5.95435
H	2.00058	-3.63239	-3.93970
H	2.20870	-3.77075	-5.67194
H	2.55043	-2.22997	-4.88884
Cl	0.25087	-0.03928	2.52444
Na	-0.97123	-2.19419	2.38988

Calculated Structure **4**: Singlet

Mo	0.02559	-0.56320	-0.23107
P	-2.61623	-0.36315	-0.38495
P	2.66068	-0.41108	-0.51751
O	-0.08424	-1.92907	-2.88125
C	-1.33908	2.51348	0.26724
C	-0.62791	2.16485	-0.88607
C	0.76087	2.15177	-0.86960
C	1.46492	2.48001	0.29195
C	0.75435	2.92481	1.40506
C	-0.63400	2.93999	1.39150
C	-2.81759	2.42936	0.26934
C	-3.50060	1.25534	-0.10004
C	-4.90227	1.28545	-0.10796
C	-5.61390	2.42367	0.24246
C	-4.93048	3.56957	0.63400
C	-3.54537	3.56472	0.64539
C	2.93782	2.33418	0.32370
C	3.58938	1.15236	-0.08653
C	4.99100	1.14059	-0.05881
C	5.73020	2.23527	0.36692
C	5.07641	3.38326	0.79731
C	3.69223	3.42435	0.77181
C	-3.65358	-1.41141	0.78037
C	-3.36692	-2.90629	0.63286
C	-3.49644	-0.88622	2.21625
C	-3.17807	-0.93412	-2.07866
C	-2.73712	0.06685	-3.14995
C	-4.65844	-1.26679	-2.27985
C	3.69131	-1.66571	0.41476
C	3.46084	-1.53186	1.91893
C	3.46741	-3.10346	-0.05633
C	3.12374	-0.77001	-2.29676
C	2.56732	0.28079	-3.25721
C	4.60817	-0.98621	-2.59420
C	-0.05822	-1.26362	-1.90170
C	0.14894	-2.46912	0.04608
H	-1.16015	1.94203	-1.80246
H	1.30255	1.91832	-1.77556
H	1.28454	3.15882	2.32099
H	-1.17584	3.19831	2.29478
H	-5.46339	0.39834	-0.37090
H	-6.69769	2.41001	0.22106
H	-5.47402	4.46260	0.92063
H	-3.00046	4.45913	0.92780
H	5.53368	0.25610	-0.36452
H	6.81310	2.18497	0.36990
H	5.64065	4.24276	1.14082
H	3.17029	4.32358	1.08117
H	-4.69872	-1.27222	0.49993
H	-2.31321	-3.16193	0.77138
H	-3.60925	-3.26821	-0.36847
H	-3.96713	-3.47865	1.34608
H	-2.48904	-0.51337	2.43739
H	-3.77614	-1.65258	2.94800
H	-4.14891	-0.02859	2.38784
H	-2.59403	-1.85132	-2.21705
H	-3.24335	1.02813	-3.01334
H	-3.00757	-0.31345	-4.13814
H	-1.65929	0.22509	-3.14669
H	-5.08022	-1.90837	-1.50398
H	-4.77022	-1.79831	-3.22881
H	-5.26515	-0.36207	-2.35236
H	4.73404	-1.41675	0.21089
H	4.13145	-2.20869	2.45659
H	2.43211	-1.77947	2.18207
H	3.64386	-0.51533	2.27446
H	2.47448	-3.45899	0.21212
H	4.19751	-3.75505	0.43266
H	3.58289	-3.22879	-1.13470
H	2.58248	-1.70415	-2.48509
H	1.48031	0.35208	-3.19999
H	2.82332	0.00936	-4.28480
H	3.00861	1.26395	-3.06201
H	5.15543	-0.04093	-2.57090
H	4.71145	-1.39392	-3.60400
H	5.09565	-1.68649	-1.91394
H	0.63609	-2.77538	1.00916
Si	-0.16966	-4.05272	-0.90851
H	-0.34296	-5.13618	0.11214
H	-1.43222	-4.04761	-1.68976
H	0.92690	-4.50835	-1.80240
B	0.39553	-2.79469	-5.10628
C	0.00167	-1.44837	-5.82931
C	-0.67897	-3.93663	-4.93819
C	1.91664	-3.12109	-4.83100
H	0.52512	-0.58617	-5.40632
H	0.32024	-1.51009	-6.87952
H	-1.07067	-1.23776	-5.83011
H	-0.36966	-4.74924	-4.27617
H	-1.63558	-3.54435	-4.58057
H	-0.87682	-4.37848	-5.92508
H	2.05136	-3.62719	-3.87002
H	2.26135	-3.83297	-5.59389
H	2.58449	-2.25609	-4.87435
Cl	0.26025	-0.04761	2.52158
Na	-0.94438	-2.21210	2.36608

Calculated Structure **5**: Singlet

Mo	0.01987	-0.55221	-0.23289
P	-2.61185	-0.35045	-0.38457
P	2.66365	-0.39131	-0.53883
O	-0.09365	-2.00332	-2.83384
C	-1.33120	2.52002	0.28550
C	-0.61632	2.17740	-0.86764
C	0.77219	2.16478	-0.84545
C	1.47266	2.48625	0.32011
C	0.75863	2.92346	1.43386
C	-0.63001	2.93852	1.41508
C	-2.80962	2.44073	0.27815
C	-3.49281	1.27074	-0.10282
C	-4.89430	1.30512	-0.12143
C	-5.60512	2.44404	0.22870
C	-4.92146	3.58591	0.63136
C	-3.53652	3.57662	0.65402
C	2.94483	2.33732	0.35401
C	3.59500	1.16163	-0.07692
C	4.99662	1.14681	-0.04663
C	5.73697	2.23181	0.40119
C	5.08455	3.37290	0.85154
C	3.70056	3.41744	0.82367
C	-3.65311	-1.38893	0.78669
C	-3.38345	-2.88644	0.64036
C	-3.48106	-0.86713	2.22104
C	-3.17618	-0.92585	-2.07566
C	-2.71870	0.06236	-3.15172
C	-4.65890	-1.24540	-2.28048
C	3.69529	-1.67182	0.35695
C	3.44342	-1.59174	1.86160
C	3.48081	-3.09000	-0.17251
C	3.11507	-0.71837	-2.32672
C	2.51128	0.31298	-3.27900
C	4.60309	-0.88042	-2.64011
C	-0.06350	-1.30665	-1.87539
C	0.13060	-2.46319	-0.01401
H	-1.14507	1.96252	-1.78793
H	1.31699	1.93831	-1.75109
H	1.28537	3.15091	2.35340
H	-1.17538	3.19200	2.31766
H	-5.45602	0.42099	-0.39261
H	-6.68872	2.43379	0.19851
H	-5.46456	4.47927	0.91768
H	-2.99098	4.46791	0.94490
H	5.53839	0.26801	-0.36960
H	6.81974	2.17942	0.40506
H	5.64975	4.22480	1.21188
H	3.17984	4.31216	1.14775
H	-4.69849	-1.23849	0.51250
H	-2.33418	-3.15448	0.78720
H	-3.62482	-3.24717	-0.36157
H	-3.99283	-3.45105	1.35183
H	-2.46009	-0.53537	2.44464
H	-3.79190	-1.62119	2.95244
H	-4.09946	0.01642	2.38849
H	-2.60197	-1.85040	-2.20559
H	-3.21753	1.02907	-3.02673
H	-2.98437	-0.32342	-4.13907
H	-1.63941	0.21112	-3.13894
H	-5.09148	-1.87136	-1.49763
H	-4.77128	-1.78917	-3.22244
H	-5.25545	-0.33542	-2.36903
H	4.74003	-1.41225	0.17754
H	4.12363	-2.26899	2.38636
H	2.41823	-1.87211	2.10381
H	3.59610	-0.58281	2.25149
H	2.45473	-3.42110	-0.02351
H	4.13593	-3.77651	0.37169
H	3.70954	-3.18953	-1.23524
H	2.60427	-1.67017	-2.51168
H	1.42471	0.36212	-3.19208
H	2.74612	0.03845	-4.31092
H	2.93739	1.30646	-3.10354
H	5.11635	0.08371	-2.61263
H	4.71249	-1.27663	-3.65385
H	5.12172	-1.56705	-1.96893
H	0.65063	-2.79515	0.92629
Si	-0.25746	-4.05786	-0.93040
H	-0.46809	-5.08847	0.13829
H	-1.52277	-4.04527	-1.70588
H	0.82371	-4.59027	-1.79967
B	0.40357	-2.86918	-5.06536
C	-0.01222	-1.53066	-5.79030
C	-0.65227	-4.02854	-4.90036
C	1.92827	-3.16648	-4.77822
H	0.46872	-0.65690	-5.34136
H	0.34295	-1.56992	-6.82964
H	-1.09025	-1.35446	-5.82349
H	-0.32467	-4.84997	-4.25843
H	-1.60699	-3.65251	-4.52064
H	-0.86256	-4.45310	-5.89218
H	2.06364	-3.64483	-3.80297
H	2.28611	-3.89466	-5.51918
H	2.58533	-2.29425	-4.84069
Cl	0.28920	-0.06049	2.51586
Na	-0.89811	-2.23434	2.33940

Calculated Structure **6**: Singlet

Mo	0.00967	-0.54093	-0.22681
P	-2.60682	-0.34653	-0.38785
P	2.66631	-0.37622	-0.54617
O	-0.09773	-2.06962	-2.78780
C	-1.32440	2.52079	0.28588
C	-0.60261	2.17503	-0.86308
C	0.78574	2.16495	-0.83044
C	1.47905	2.49125	0.33824
C	0.75836	2.92941	1.44678
C	-0.63055	2.94169	1.41868
C	-2.80269	2.44702	0.26561
C	-3.48545	1.27905	-0.12136
C	-4.88652	1.31826	-0.15454
C	-5.59693	2.46028	0.18666
C	-4.91369	3.60028	0.59526
C	-3.52906	3.58615	0.63243
C	2.95039	2.34080	0.37842
C	3.60029	1.16861	-0.06338
C	5.00180	1.15143	-0.02853
C	5.74213	2.23032	0.43401
C	5.08981	3.36730	0.89490
C	3.70603	3.41440	0.86263
C	-3.65708	-1.36929	0.79007
C	-3.40215	-2.86951	0.65415
C	-3.47398	-0.84669	2.22103
C	-3.16814	-0.93323	-2.07613
C	-2.69519	0.04101	-3.15820
C	-4.65184	-1.24450	-2.28705
C	3.69954	-1.67750	0.31813
C	3.43009	-1.64292	1.82172
C	3.49471	-3.07726	-0.26321
C	3.10801	-0.68227	-2.34054
C	2.46547	0.32787	-3.28964
C	4.59769	-0.79902	-2.66517
C	-0.06438	-1.35953	-1.83817
C	0.12442	-2.45819	-0.05848
H	-1.12522	1.96460	-1.78783
H	1.33711	1.94091	-1.73242
H	1.27870	3.15918	2.36930
H	-1.18242	3.19749	2.31667
H	-5.44855	0.43577	-0.42977
H	-6.68018	2.45370	0.14519
H	-5.45667	4.49586	0.87476
H	-2.98331	4.47586	0.92767
H	5.54366	0.27640	-0.36137
H	6.82481	2.17653	0.44026
H	5.65513	4.21442	1.26615
H	3.18560	4.30656	1.19399
H	-4.70157	-1.20795	0.51790
H	-2.35861	-3.14574	0.82424
H	-3.63058	-3.23468	-0.34913
H	-4.02724	-3.42356	1.36017
H	-2.43710	-0.57758	2.45410
H	-3.83604	-1.57677	2.95248
H	-4.04015	0.07403	2.37402
H	-2.60111	-1.86352	-2.19467
H	-3.18613	1.01323	-3.04487
H	-2.95788	-0.35073	-4.14400
H	-1.61460	0.18012	-3.13786
H	-5.09506	-1.85377	-1.49694
H	-4.76153	-1.80300	-3.22072
H	-5.24041	-0.33153	-2.39543
H	4.74566	-1.40949	0.16060
H	4.11693	-2.32125	2.33616
H	2.40798	-1.94835	2.04535
H	3.55817	-0.64195	2.23978
H	2.45025	-3.38242	-0.22337
H	4.07581	-3.79677	0.32084
H	3.82215	-3.15623	-1.30141
H	2.62409	-1.64905	-2.52098
H	1.37998	0.35780	-3.18001
H	2.68450	0.04671	-4.32330
H	2.87672	1.33076	-3.13400
H	5.08239	0.17970	-2.63275
H	4.71296	-1.18506	-3.68220
H	5.14065	-1.47371	-2.00111
H	0.70065	-2.80282	0.84613
Si	-0.32076	-4.06645	-0.92478
H	-0.55041	-5.04363	0.19027
H	-1.58957	-4.05788	-1.69323
H	0.74675	-4.65878	-1.77117
B	0.39194	-2.90642	-5.03964
C	-0.03494	-1.56596	-5.75427
C	-0.65668	-4.07280	-4.87995
C	1.91889	-3.19271	-4.75297
H	0.42063	-0.69111	-5.28162
H	0.34315	-1.58168	-6.78606
H	-1.11500	-1.40814	-5.80697
H	-0.32206	-4.90060	-4.25000
H	-1.60997	-3.70396	-4.48955
H	-0.87329	-4.48594	-5.87520
H	2.05595	-3.66066	-3.77273
H	2.28145	-3.92601	-5.48637
H	2.57082	-2.31702	-4.82261
Cl	0.30959	-0.05752	2.51795
Na	-0.82009	-2.26276	2.32582

Calculated Structure **7**: Singlet

Mo	0.03296	-0.58417	-0.21803
P	-2.56107	-0.73031	-0.17604
P	2.67479	-0.51335	-0.13771
O	0.11022	-1.82380	-3.05755
C	-1.39421	2.23592	-0.02362
C	-0.73497	1.51016	-1.07858
C	0.67435	1.54337	-1.13970
C	1.41125	2.34666	-0.20395
C	0.75393	3.05657	0.75751
C	-0.66325	2.98581	0.85336
C	-2.85771	2.11251	0.11798
C	-3.50528	0.86385	0.05348
C	-4.89631	0.83805	0.22683
C	-5.63335	1.99370	0.44255
C	-4.98520	3.22226	0.50185
C	-3.61116	3.27242	0.34237
C	2.88294	2.32039	-0.29444
C	3.56478	1.09742	-0.38408
C	4.96023	1.11877	-0.48547
C	5.66976	2.31060	-0.49985
C	4.98763	3.51951	-0.39037
C	3.60611	3.51912	-0.28894
C	-3.47670	-1.77864	1.09195
C	-3.13533	-3.26201	0.98037
C	-3.28553	-1.26333	2.51817
C	-3.27107	-1.37414	-1.79651
C	-3.02951	-0.38128	-2.93635
C	-4.74367	-1.79405	-1.81541
C	3.62934	-1.05220	1.39211
C	3.64892	0.04404	2.46328
C	3.07668	-2.34611	1.99351
C	3.37080	-1.59768	-1.52075
C	3.46814	-0.80183	-2.82406
C	4.65814	-2.37970	-1.25169
C	0.09237	-1.37286	-1.96781
C	0.28927	-2.61273	-0.41090
H	-1.30977	1.27492	-1.96251
H	1.17008	1.27047	-2.06416
H	1.31411	3.61919	1.49623
H	-1.16306	3.48541	1.67605
H	-5.43311	-0.10069	0.20797
H	-6.70876	1.93180	0.56472
H	-5.54839	4.13411	0.66494
H	-3.09522	4.22589	0.36713
H	5.51230	0.18810	-0.53468
H	6.75028	2.29632	-0.58638
H	5.53196	4.45705	-0.39476
H	3.06058	4.45456	-0.22678
H	-4.53869	-1.68763	0.86225
H	-2.06641	-3.45527	1.10794
H	-3.39958	-3.68091	0.00853
H	-3.67032	-3.82996	1.74682
H	-2.25385	-1.34879	2.86268
H	-3.92462	-1.82939	3.20227
H	-3.54293	-0.20654	2.60894
H	-2.65979	-2.25778	-1.99483
H	-3.46724	0.59665	-2.71306
H	-3.50544	-0.75428	-3.84600
H	-1.97061	-0.26247	-3.16050
H	-5.02852	-2.46778	-1.00621
H	-4.94198	-2.32049	-2.75301
H	-5.40461	-0.92521	-1.79583
H	4.65730	-1.23427	1.06535
H	4.12603	-0.34332	3.36906
H	2.63552	0.35564	2.72199
H	4.20901	0.92219	2.14090
H	2.17231	-2.10661	2.56103
H	3.79272	-2.76458	2.70601
H	2.85177	-3.11608	1.25163
H	2.58230	-2.33603	-1.68015
H	2.51622	-0.32906	-3.07483
H	3.71908	-1.48058	-3.64273
H	4.23722	-0.02879	-2.77891
H	5.53697	-1.73817	-1.16274
H	4.84283	-3.05201	-2.09428
H	4.59815	-2.99686	-0.35317
H	1.35049	-2.91266	-0.37515
Si	-0.44073	-4.16953	-1.12801
H	-0.45449	-5.20397	-0.04589
H	-1.82828	-4.09964	-1.64219
H	0.40488	-4.71993	-2.21762
B	0.10666	-0.82783	-5.53277
C	0.38286	0.63382	-5.00674
C	-1.36844	-1.28080	-5.85801
C	1.29028	-1.78385	-5.92963
H	1.41454	0.83204	-4.70653
H	0.13755	1.34110	-5.81107
H	-0.28135	0.90451	-4.17844
H	-1.65990	-2.03140	-5.11237
H	-2.11352	-0.48194	-5.83364
H	-1.42775	-1.78667	-6.82784
H	1.00691	-2.83882	-5.96409
H	1.60644	-1.50959	-6.94714
H	2.16972	-1.67398	-5.29341
Cl	0.02052	-0.00497	2.41951
Na	-0.09741	-2.55581	2.10971

Calculated Structure **8**: Singlet

Mo	0.02676	-0.52466	-0.32019
P	-2.57325	-0.68330	-0.19999
P	2.66699	-0.44807	-0.25750
O	-0.21239	-1.85124	-3.11923
C	-1.41494	2.28592	0.04207
C	-0.75966	1.63159	-1.05724
C	0.64626	1.66884	-1.12994
C	1.39098	2.41194	-0.15126
C	0.73525	3.06696	0.85103
C	-0.67876	2.98952	0.95421
C	-2.87639	2.14750	0.19700
C	-3.51573	0.89675	0.10913
C	-4.90240	0.85521	0.31077
C	-5.64264	1.99913	0.57300
C	-5.00262	3.23060	0.65273
C	-3.63209	3.29533	0.46888
C	2.86504	2.39080	-0.22488
C	3.55269	1.17575	-0.34753
C	4.95118	1.19771	-0.39676
C	5.65929	2.38776	-0.33465
C	4.97063	3.59177	-0.20388
C	3.58686	3.58858	-0.14783
C	-3.43858	-1.77741	1.06156
C	-3.09165	-3.25301	0.88793
C	-3.20870	-1.31109	2.49871
C	-3.32243	-1.27378	-1.82071
C	-3.12972	-0.22419	-2.91765
C	-4.78878	-1.71454	-1.81160
C	3.60978	-1.13816	1.22659
C	3.71181	-0.11685	2.36742
C	3.00908	-2.43365	1.78387
C	3.36768	-1.37222	-1.75975
C	3.83394	-0.41952	-2.86658
C	4.44734	-2.41778	-1.47906
C	-0.03981	-1.33447	-2.03777
C	0.31865	-2.55879	-0.62975
H	-1.34036	1.41292	-1.94203
H	1.13095	1.43046	-2.06883
H	1.29964	3.58921	1.61579
H	-1.17367	3.44276	1.80612
H	-5.43286	-0.08659	0.27605
H	-6.71485	1.92566	0.71509
H	-5.56886	4.13328	0.85195
H	-3.12163	4.25113	0.51269
H	5.50238	0.26504	-0.46425
H	6.74233	2.37789	-0.38073
H	5.51384	4.52856	-0.15302
H	3.03999	4.52146	-0.06337
H	-4.50704	-1.68585	0.86406
H	-2.01590	-3.43967	0.95494
H	-3.40036	-3.64530	-0.08156
H	-3.58151	-3.84910	1.66301
H	-2.17389	-1.43750	2.81932
H	-3.84993	-1.88301	3.17577
H	-3.43772	-0.25183	2.62817
H	-2.70548	-2.13764	-2.08144
H	-3.58360	0.73165	-2.63811
H	-3.61834	-0.56724	-3.83201
H	-2.08001	-0.07184	-3.16093
H	-5.04159	-2.42185	-1.02045
H	-5.00461	-2.20928	-2.76231
H	-5.46151	-0.85748	-1.74252
H	4.61864	-1.36030	0.86915
H	4.16421	-0.59904	3.23980
H	2.72316	0.24276	2.65740
H	4.32839	0.74182	2.10541
H	2.18501	-2.16933	2.45371
H	3.75164	-2.95200	2.39621
H	2.66356	-3.13133	1.01830
H	2.49201	-1.89871	-2.14730
H	3.15976	0.42593	-3.00504
H	3.88343	-0.96011	-3.81429
H	4.82513	-0.01408	-2.66053
H	5.38729	-1.96221	-1.15571
H	4.65778	-2.96562	-2.40187
H	4.14987	-3.14954	-0.72519
H	1.38783	-2.81937	-0.70970
Si	-0.44867	-4.11678	-1.31693
H	-0.40047	-5.13553	-0.21780
H	-1.86373	-4.03582	-1.73935
H	0.34425	-4.66918	-2.43988
B	0.14035	-1.31570	-4.83014
C	0.47885	0.24143	-4.66962
C	-1.22316	-1.68228	-5.58301
C	1.36913	-2.29160	-5.15338
H	1.38857	0.42808	-4.09203
H	0.65214	0.66864	-5.66509
H	-0.33220	0.83029	-4.22373
H	-1.60661	-2.66521	-5.28659
H	-2.02552	-0.95122	-5.45090
H	-1.02771	-1.74080	-6.66111
H	1.07079	-3.34493	-5.18132
H	1.78398	-2.05069	-6.14030
H	2.19220	-2.20372	-4.43635
Cl	0.08738	-0.11761	2.32870
Na	0.00279	-2.66475	1.88722

Calculated Structure **9**: Singlet

Mo	0.07299	-0.50126	-0.30811
P	-2.56316	-0.58042	-0.26969
P	2.70627	-0.52024	-0.19796
O	0.30352	-1.77790	-3.17193
C	-1.33483	2.30232	0.04877
C	-0.64697	1.64642	-1.03660
C	0.76282	1.65095	-1.04552
C	1.47834	2.34279	-0.00401
C	0.79769	2.95774	1.00390
C	-0.62671	2.92719	1.03366
C	-2.80871	2.24510	0.06928
C	-3.47494	1.03146	-0.14010
C	-4.87481	1.02974	-0.14775
C	-5.60253	2.19205	0.05381
C	-4.93338	3.39230	0.28300
C	-3.54899	3.41425	0.28813
C	2.95143	2.30901	-0.05215
C	3.62286	1.09280	-0.24302
C	5.02078	1.10699	-0.30006
C	5.74019	2.28669	-0.17602
C	5.06681	3.48738	0.03118
C	3.68282	3.49346	0.09221
C	-3.50983	-1.47620	1.09571
C	-2.91199	-2.84432	1.44100
C	-3.62019	-0.64214	2.37843
C	-3.26659	-1.27221	-1.88765
C	-3.73111	-0.17515	-2.85421
C	-4.36212	-2.33120	-1.75653
C	3.62100	-1.24986	1.27221
C	3.60079	-0.30695	2.47994
C	3.08548	-2.62547	1.67650
C	3.40390	-1.44928	-1.68358
C	3.48124	-0.51888	-2.89589
C	4.70761	-2.23068	-1.50555
C	0.20225	-1.33855	-2.03209
C	0.28849	-2.57557	-0.72735
H	-1.18484	1.46768	-1.95798
H	1.28811	1.45505	-1.97148
H	1.34095	3.43497	1.81220
H	-1.15237	3.37870	1.86808
H	-5.41225	0.09952	-0.30020
H	-6.68602	2.16331	0.03589
H	-5.49188	4.30759	0.44247
H	-3.01714	4.34812	0.43461
H	5.56754	0.18095	-0.42471
H	6.82256	2.26815	-0.23267
H	5.61955	4.41424	0.13368
H	3.14401	4.42489	0.22863
H	-4.51612	-1.64095	0.70401
H	-2.15588	-2.70260	2.22028
H	-2.48551	-3.36783	0.58240
H	-3.67784	-3.49363	1.87267
H	-2.63396	-0.33457	2.72908
H	-4.08207	-1.25128	3.16204
H	-4.23240	0.24864	2.24648
H	-2.39215	-1.74408	-2.33776
H	-4.73231	0.17946	-2.60497
H	-3.75660	-0.57705	-3.86972
H	-3.07511	0.69459	-2.86317
H	-4.10380	-3.14438	-1.07679
H	-4.54172	-2.77491	-2.74006
H	-5.30822	-1.89624	-1.42254
H	4.65856	-1.36909	0.94733
H	4.08559	-0.79639	3.33032
H	2.57768	-0.06350	2.77074
H	4.13585	0.62223	2.28111
H	2.17534	-2.48491	2.26648
H	3.80621	-3.13138	2.32439
H	2.88307	-3.28256	0.82666
H	2.62982	-2.18245	-1.91729
H	2.52470	-0.03012	-3.09287
H	3.72223	-1.10431	-3.78542
H	4.24684	0.24960	-2.77104
H	5.57723	-1.58467	-1.37412
H	4.88660	-2.81604	-2.41156
H	4.67459	-2.93169	-0.66935
H	1.33461	-2.91255	-0.74746
Si	-0.62222	-4.05165	-1.37780
H	-0.63389	-5.06144	-0.25905
H	-2.04479	-3.83673	-1.72154
H	0.05345	-4.71210	-2.51810
B	-0.03908	-1.11355	-4.71665
C	-0.37379	0.44003	-4.47916
C	-1.27996	-2.03568	-5.17297
C	1.30040	-1.39358	-5.56375
H	-1.28861	0.60321	-3.90312
H	0.43924	0.99333	-3.99174
H	-0.53058	0.92482	-5.45007
H	-0.99319	-3.08813	-5.28091
H	-2.13378	-2.00272	-4.48585
H	-1.65270	-1.70693	-6.15084
H	1.70940	-2.39380	-5.37764
H	1.06457	-1.35026	-6.63408
H	2.10032	-0.66619	-5.39411
Cl	-0.00291	-0.58773	2.36623
Na	-0.01103	-3.06661	1.64015

Calculated Structure **10**: Singlet

Mo	0.06455	-0.45395	-0.28236
P	-2.56123	-0.55249	-0.26427
P	2.71377	-0.51724	-0.18337
O	0.29199	-1.77994	-3.14535
C	-1.33011	2.31968	0.01181
C	-0.64408	1.63512	-1.06296
C	0.77079	1.63028	-1.06846
C	1.48614	2.34326	-0.03440
C	0.80646	2.97402	0.96112
C	-0.62191	2.95178	0.98842
C	-2.80438	2.27259	0.03385
C	-3.47555	1.05737	-0.14650
C	-4.87511	1.05892	-0.14500
C	-5.59755	2.22770	0.03768
C	-4.92342	3.43054	0.23572
C	-3.53891	3.44879	0.23131
C	2.95982	2.31113	-0.07099
C	3.63647	1.09180	-0.21742
C	5.03545	1.10722	-0.24349
C	5.74997	2.29181	-0.13842
C	5.07074	3.49668	0.01670
C	3.68594	3.50111	0.05155
C	-3.50935	-1.44973	1.09683
C	-2.93000	-2.82963	1.42601
C	-3.60315	-0.62364	2.38549
C	-3.25488	-1.24998	-1.88306
C	-3.72855	-0.15692	-2.85014
C	-4.34611	-2.31408	-1.75353
C	3.62656	-1.27966	1.26796
C	3.58091	-0.37610	2.50370
C	3.11253	-2.67830	1.61507
C	3.40048	-1.43018	-1.68303
C	3.43049	-0.49499	-2.89341
C	4.73287	-2.16912	-1.53643
C	0.20442	-1.40413	-1.97020
C	0.27899	-2.58479	-0.74934
H	-1.17951	1.46238	-1.98670
H	1.29668	1.43519	-1.99411
H	1.34987	3.46457	1.76124
H	-1.14650	3.42218	1.81297
H	-5.41637	0.12787	-0.27732
H	-6.68120	2.20210	0.02801
H	-5.47839	4.35061	0.37897
H	-3.00326	4.38380	0.35457
H	5.58728	0.17983	-0.32715
H	6.83337	2.27356	-0.17007
H	5.61971	4.42751	0.10176
H	3.14288	4.43456	0.15187
H	-4.51949	-1.59733	0.70818
H	-2.16651	-2.70720	2.20041
H	-2.51695	-3.34925	0.55851
H	-3.70455	-3.47232	1.85212
H	-2.61125	-0.34008	2.74028
H	-4.07836	-1.22825	3.16458
H	-4.19654	0.28068	2.25854
H	-2.37694	-1.71635	-2.33232
H	-4.73590	0.18280	-2.60426
H	-3.74352	-0.55777	-3.86622
H	-3.08569	0.72236	-2.85492
H	-4.08683	-3.12799	-1.07549
H	-4.52298	-2.75628	-2.73826
H	-5.29396	-1.88239	-1.42024
H	4.66876	-1.37093	0.94916
H	4.08362	-0.87504	3.33797
H	2.55236	-0.17214	2.80412
H	4.08698	0.57450	2.33039
H	2.17393	-2.58150	2.16678
H	3.82143	-3.18212	2.27763
H	2.96445	-3.31601	0.73975
H	2.64261	-2.18548	-1.90067
H	2.45167	-0.05429	-3.09038
H	3.69896	-1.06579	-3.78440
H	4.16007	0.30792	-2.76622
H	5.58301	-1.49147	-1.44329
H	4.90140	-2.75800	-2.44213
H	4.75198	-2.86186	-0.69326
H	1.32576	-2.91326	-0.71929
Si	-0.63455	-4.07028	-1.35597
H	-0.72653	-5.03696	-0.19759
H	-2.03437	-3.84058	-1.77317
H	0.07771	-4.80557	-2.42554
B	-0.03457	-1.10257	-4.64686
C	-0.37914	0.45521	-4.43831
C	-1.27383	-2.01817	-5.13606
C	1.29990	-1.37134	-5.51461
H	-1.30978	0.62709	-3.89144
H	0.41864	1.02447	-3.94448
H	-0.51349	0.91932	-5.42273
H	-0.98180	-3.06753	-5.26201
H	-2.13466	-2.00439	-4.45665
H	-1.63880	-1.67161	-6.11068
H	1.73803	-2.35594	-5.31030
H	1.04403	-1.36239	-6.58108
H	2.08540	-0.62089	-5.38079
Cl	0.00582	-0.75925	2.34920
Na	-0.04671	-3.20185	1.56591

Calculated Structure **11**: Singlet

Mo	0.14216	-0.49342	-0.53709
P	-2.55949	-0.40481	-0.43734
P	2.70323	-0.45431	-0.57944
O	0.30117	-2.68535	-2.70878
C	-1.36625	2.46766	-0.14516
C	-0.51558	1.91050	-1.13748
C	0.86686	1.90204	-0.94722
C	1.41359	2.36746	0.28199
C	0.57336	2.91498	1.22231
C	-0.81855	2.98503	1.00130
C	-2.82128	2.43260	-0.39255
C	-3.45441	1.21104	-0.66037
C	-4.83821	1.21226	-0.86406
C	-5.57448	2.38849	-0.83485
C	-4.93589	3.59714	-0.57288
C	-3.56804	3.61362	-0.34723
C	2.85794	2.20566	0.53774
C	3.54777	1.01740	0.21431
C	4.91442	0.96299	0.52215
C	5.58519	2.02433	1.11411
C	4.89595	3.19021	1.42166
C	3.54456	3.27019	1.13390
C	-3.51441	-0.84586	1.12980
C	-3.03485	-2.13059	1.80981
C	-3.47514	0.29924	2.15035
C	-3.31715	-1.49336	-1.79416
C	-3.76406	-0.72645	-3.05598
C	-4.43490	-2.44576	-1.36117
C	3.62621	-1.89145	0.19616
C	3.23236	-2.09328	1.65931
C	3.52837	-3.16387	-0.67172
C	3.51626	-0.49412	-2.28325
C	3.17520	0.69961	-3.17860
C	5.04240	-0.64721	-2.30480
C	0.27817	-2.10840	-1.59422
C	0.19209	-2.81798	-0.16276
H	-0.92759	1.72226	-2.12122
H	1.52204	1.77711	-1.79448
H	0.97416	3.22990	2.17891
H	-1.46628	3.38679	1.77304
H	-5.36023	0.27612	-1.02398
H	-6.64481	2.36055	-1.00524
H	-5.50261	4.52087	-0.54724
H	-3.05542	4.54873	-0.14856
H	5.49225	0.07760	0.29887
H	6.64482	1.93833	1.32681
H	5.40874	4.03193	1.87289
H	2.99947	4.18323	1.34664
H	-4.54960	-0.98837	0.80738
H	-2.64797	-2.87891	1.11645
H	-3.85189	-2.59255	2.36984
H	-2.27084	-1.86087	2.54476
H	-2.44321	0.58287	2.37411
H	-3.93917	-0.03565	3.08317
H	-4.01677	1.18110	1.80881
H	-2.45780	-2.10553	-2.08044
H	-4.82663	-0.48106	-3.01464
H	-3.60444	-1.35494	-3.93435
H	-3.22896	0.20831	-3.22056
H	-4.17800	-3.05661	-0.49558
H	-4.65178	-3.12945	-2.18714
H	-5.36142	-1.91181	-1.13427
H	4.67814	-1.61689	0.21591
H	3.87248	-2.85602	2.11148
H	2.19734	-2.41285	1.75606
H	3.33169	-1.17022	2.23368
H	2.61720	-3.23243	-1.26644
H	3.57402	-4.05604	-0.04073
H	4.35887	-3.22350	-1.37692
H	3.06838	-1.39050	-2.72511
H	2.11657	0.77357	-3.41696
H	3.69920	0.58996	-4.13174
H	3.51905	1.63756	-2.73046
H	5.53052	0.28874	-2.02368
H	5.35100	-0.87811	-3.32806
H	5.43232	-1.44157	-1.66983
H	1.19778	-3.12973	0.12007
Si	-0.83135	-4.34320	-0.31344
H	-1.13173	-4.85338	1.07522
H	-2.15177	-4.11761	-0.94580
H	-0.15407	-5.46847	-1.00033
B	0.07609	-1.87187	-4.08978
C	-0.28084	-0.35503	-3.61229
C	-1.15553	-2.64655	-4.80040
C	1.43259	-2.00305	-4.96054
H	0.40217	-0.03697	-2.79176
H	-0.12611	0.39888	-4.39350
H	-1.30851	-0.25225	-3.26575
H	-0.84441	-3.61781	-5.20184
H	-1.99534	-2.84416	-4.12291
H	-1.55239	-2.06868	-5.64454
H	1.80132	-3.03551	-4.97290
H	1.22131	-1.73888	-6.00402
H	2.26335	-1.36199	-4.64814
Cl	0.27058	-0.16821	2.20548
Na	-0.22681	-2.60977	2.18021

Calculated Structure **12**: Singlet

Mo	0.14166	-0.49344	-0.54147
P	-2.56211	-0.39607	-0.44301
P	2.69985	-0.45272	-0.59404
O	0.28414	-2.70479	-2.68309
C	-1.35779	2.47374	-0.14429
C	-0.50173	1.92977	-1.13776
C	0.87869	1.91768	-0.93846
C	1.41940	2.36485	0.29751
C	0.57479	2.90372	1.24077
C	-0.81509	2.97775	1.01237
C	-2.81248	2.44255	-0.40009
C	-3.44931	1.22327	-0.67330
C	-4.83135	1.23032	-0.88864
C	-5.56280	2.40949	-0.86536
C	-4.92173	3.61483	-0.59537
C	-3.55570	3.62574	-0.35785
C	2.86283	2.19359	0.55534
C	3.54892	1.00793	0.21413
C	4.91595	0.94494	0.51734
C	5.59203	1.99682	1.11942
C	4.90677	3.15972	1.44643
C	3.55413	3.24742	1.16536
C	-3.51789	-0.83216	1.12621
C	-3.03743	-2.11833	1.80306
C	-3.46898	0.31095	2.14804
C	-3.32295	-1.48937	-1.79541
C	-3.79076	-0.72692	-3.05182
C	-4.42982	-2.45127	-1.35528
C	3.62887	-1.89346	0.16947
C	3.24283	-2.10354	1.63362
C	3.52753	-3.16363	-0.70212
C	3.51244	-0.47998	-2.29923
C	3.14687	0.70591	-3.19509
C	5.04136	-0.60228	-2.32565
C	0.28492	-2.14900	-1.54739
C	0.19658	-2.82477	-0.21115
H	-0.90909	1.74533	-2.12388
H	1.53918	1.79048	-1.78050
H	0.97077	3.20560	2.20376
H	-1.46694	3.37131	1.78520
H	-5.35566	0.29649	-1.05302
H	-6.63140	2.38622	-1.04637
H	-5.48499	4.54063	-0.57258
H	-3.04152	4.55847	-0.15211
H	5.48897	0.05947	0.28132
H	6.65235	1.90561	1.32538
H	5.42324	3.99387	1.90717
H	3.01192	4.15872	1.39294
H	-4.55501	-0.97043	0.80835
H	-2.65229	-2.86379	1.10593
H	-3.85322	-2.58331	2.36223
H	-2.27255	-1.84897	2.53813
H	-2.43394	0.59173	2.36308
H	-3.92569	-0.02442	3.08428
H	-4.01159	1.19453	1.81235
H	-2.46065	-2.09310	-2.09064
H	-4.85624	-0.49729	-3.00194
H	-3.62877	-1.35202	-3.93197
H	-3.27130	0.21606	-3.21916
H	-4.16187	-3.06056	-0.49205
H	-4.64657	-3.13596	-2.18055
H	-5.35945	-1.92579	-1.12123
H	4.68089	-1.61591	0.18482
H	3.88699	-2.86691	2.07914
H	2.20856	-2.42556	1.73751
H	3.34288	-1.18246	2.21139
H	2.61005	-3.23712	-1.28614
H	3.58725	-4.05725	-0.07415
H	4.34930	-3.21678	-1.41769
H	3.07964	-1.38446	-2.73939
H	2.08594	0.76077	-3.42712
H	3.66712	0.60390	-4.15126
H	3.47611	1.65022	-2.74944
H	5.51289	0.34316	-2.04821
H	5.35149	-0.82872	-3.34958
H	5.44858	-1.38788	-1.69051
H	1.18801	-3.12427	0.13350
Si	-0.83744	-4.35443	-0.30415
H	-1.11396	-4.81621	1.10627
H	-2.16490	-4.14133	-0.92325
H	-0.16914	-5.49929	-0.96469
B	0.05658	-1.87733	-4.03737
C	-0.29839	-0.36501	-3.53510
C	-1.17814	-2.63439	-4.76631
C	1.40343	-1.99199	-4.92944
H	0.38513	-0.06953	-2.70160
H	-0.12496	0.40832	-4.29329
H	-1.32868	-0.25957	-3.20140
H	-0.86262	-3.59088	-5.19906
H	-2.01457	-2.85922	-4.09318
H	-1.58096	-2.03369	-5.59162
H	1.76824	-3.02548	-4.96595
H	1.17972	-1.70834	-5.96527
H	2.24111	-1.36060	-4.61730
Cl	0.29610	-0.17888	2.20969
Na	-0.23373	-2.61089	2.14581

Calculated Structure **13**: Singlet

Mo	0.13384	-0.50141	-0.55911
P	-2.56499	-0.37882	-0.42948
P	2.69031	-0.44306	-0.60698
O	0.28235	-2.73281	-2.67179
C	-1.35478	2.47901	-0.14556
C	-0.49603	1.93325	-1.13564
C	0.88255	1.92042	-0.92895
C	1.41931	2.36604	0.30866
C	0.57236	2.90683	1.24939
C	-0.81642	2.98328	1.01332
C	-2.80833	2.45720	-0.40746
C	-3.45232	1.24177	-0.67622
C	-4.83421	1.25600	-0.89457
C	-5.55877	2.43980	-0.87664
C	-4.91027	3.64228	-0.60976
C	-3.54442	3.64547	-0.37085
C	2.86249	2.19123	0.57003
C	3.54538	1.00679	0.21935
C	4.91189	0.93738	0.52370
C	5.58952	1.98082	1.13907
C	4.90685	3.14242	1.47740
C	3.55533	3.23729	1.19277
C	-3.49842	-0.81383	1.15965
C	-2.99954	-2.09414	1.83829
C	-3.45477	0.33329	2.17822
C	-3.32675	-1.49615	-1.76789
C	-3.80004	-0.74659	-3.02987
C	-4.43030	-2.45866	-1.31864
C	3.62318	-1.89258	0.14038
C	3.25108	-2.11475	1.60610
C	3.51128	-3.15898	-0.73555
C	3.52354	-0.46163	-2.30182
C	3.14490	0.71391	-3.20524
C	5.05447	-0.55617	-2.31024
C	0.30949	-2.19281	-1.51746
C	0.20310	-2.82626	-0.27348
H	-0.89827	1.75532	-2.12468
H	1.54650	1.79178	-1.76724
H	0.96498	3.20871	2.21377
H	-1.47156	3.37995	1.78167
H	-5.36406	0.32450	-1.05545
H	-6.62741	2.42255	-1.05849
H	-5.46754	4.57190	-0.58999
H	-3.02474	4.57564	-0.16725
H	5.48447	0.05405	0.27780
H	6.64922	1.88400	1.34607
H	5.42483	3.96967	1.94890
H	3.01519	4.14779	1.42798
H	-4.53724	-0.96511	0.85467
H	-2.59819	-2.83324	1.14251
H	-3.80858	-2.57455	2.39431
H	-2.24246	-1.81376	2.57679
H	-2.42276	0.63411	2.37821
H	-3.89208	-0.00912	3.12144
H	-4.01873	1.20581	1.84979
H	-2.46228	-2.10054	-2.05688
H	-4.86346	-0.50899	-2.97256
H	-3.65037	-1.38267	-3.90423
H	-3.27549	0.19100	-3.21220
H	-4.15981	-3.05891	-0.45017
H	-4.64549	-3.15208	-2.13705
H	-5.36205	-1.93491	-1.08904
H	4.67539	-1.61479	0.14817
H	3.91209	-2.86813	2.04395
H	2.22407	-2.45911	1.71854
H	3.33767	-1.19446	2.18738
H	2.58396	-3.23268	-1.30433
H	3.58645	-4.05590	-0.11364
H	4.31970	-3.20500	-1.46640
H	3.11047	-1.37540	-2.74070
H	2.08235	0.75598	-3.43171
H	3.66289	0.61014	-4.16257
H	3.46685	1.66428	-2.76707
H	5.50495	0.40089	-2.03663
H	5.38149	-0.78790	-3.32793
H	5.46821	-1.32638	-1.66031
H	1.16987	-3.09844	0.15571
Si	-0.83672	-4.36316	-0.32717
H	-1.09961	-4.78037	1.10113
H	-2.16811	-4.16042	-0.94143
H	-0.16912	-5.52513	-0.95674
B	0.05439	-1.89105	-4.00206
C	-0.29696	-0.38422	-3.47256
C	-1.18358	-2.62632	-4.74969
C	1.39225	-1.98726	-4.91152
H	0.39984	-0.10913	-2.63716
H	-0.11597	0.40665	-4.21077
H	-1.32646	-0.27926	-3.14058
H	-0.86726	-3.56731	-5.21487
H	-2.01390	-2.87678	-4.07892
H	-1.59388	-2.00062	-5.55261
H	1.74822	-3.02207	-4.98206
H	1.16340	-1.66952	-5.93652
H	2.23748	-1.37365	-4.58720
Cl	0.31154	-0.20658	2.18755
Na	-0.26932	-2.62564	2.10292

Calculated Structure **14**: Singlet

Mo	0.14194	-0.45962	-0.57046
P	-2.56249	-0.38408	-0.44473
P	2.70092	-0.44328	-0.59445
O	0.20344	-2.71964	-2.65885
C	-1.34416	2.46680	-0.12050
C	-0.48755	1.92617	-1.12198
C	0.89521	1.91965	-0.92092
C	1.43229	2.36242	0.32062
C	0.58948	2.89041	1.26806
C	-0.80279	2.96165	1.03863
C	-2.80019	2.44645	-0.37430
C	-3.44862	1.23453	-0.65460
C	-4.83221	1.24999	-0.85774
C	-5.55655	2.43313	-0.81800
C	-4.90525	3.63201	-0.54360
C	-3.53717	3.63329	-0.31689
C	2.87585	2.19309	0.57279
C	3.56034	1.01015	0.22000
C	4.92934	0.94670	0.51575
C	5.60769	1.99565	1.12070
C	4.92295	3.15592	1.45887
C	3.56888	3.24368	1.18593
C	-3.50461	-0.84196	1.12624
C	-3.02597	-2.14737	1.77183
C	-3.44906	0.28268	2.16795
C	-3.32375	-1.48334	-1.79055
C	-3.82002	-0.72230	-3.03625
C	-4.41061	-2.46438	-1.34243
C	3.62992	-1.88387	0.18030
C	3.24712	-2.09561	1.64616
C	3.55350	-3.16200	-0.68042
C	3.52229	-0.48108	-2.29375
C	3.13422	0.68691	-3.20265
C	5.05205	-0.58336	-2.32110
C	0.31081	-2.19867	-1.49264
C	0.22719	-2.80504	-0.34576
H	-0.89249	1.77679	-2.11494
H	1.55670	1.82039	-1.76652
H	0.98423	3.18615	2.23318
H	-1.45586	3.35022	1.81305
H	-5.36257	0.31979	-1.02468
H	-6.62684	2.41811	-0.98928
H	-5.46259	4.56101	-0.50806
H	-3.01628	4.56125	-0.10650
H	5.50349	0.06456	0.27027
H	6.66947	1.90449	1.31939
H	5.44149	3.98786	1.92134
H	3.02661	4.15269	1.42148
H	-4.54432	-0.97039	0.81363
H	-2.59033	-2.85125	1.05879
H	-3.85457	-2.66116	2.26518
H	-2.30585	-1.89809	2.55799
H	-2.41333	0.55195	2.39140
H	-3.91387	-0.06339	3.09642
H	-3.98327	1.17556	1.84321
H	-2.45584	-2.07274	-2.10015
H	-4.88383	-0.49208	-2.96099
H	-3.67931	-1.34898	-3.91863
H	-3.30322	0.21966	-3.21722
H	-4.11864	-3.08464	-0.49472
H	-4.63703	-3.13843	-2.17383
H	-5.34085	-1.95299	-1.08102
H	4.67930	-1.59667	0.19941
H	3.93187	-2.81496	2.10409
H	2.23470	-2.48161	1.76188
H	3.28995	-1.16387	2.21331
H	2.61788	-3.28539	-1.22521
H	3.68560	-4.04620	-0.04975
H	4.34574	-3.17987	-1.43012
H	3.10076	-1.39695	-2.72143
H	2.06802	0.73170	-3.41224
H	3.63613	0.57193	-4.16717
H	3.46589	1.64003	-2.77815
H	5.51154	0.37113	-2.05495
H	5.36443	-0.81797	-3.34256
H	5.46991	-1.35602	-1.67640
H	1.16644	-2.97249	0.18093
Si	-0.75118	-4.39132	-0.37558
H	-0.98380	-4.78474	1.06354
H	-2.09216	-4.23993	-0.98094
H	-0.03769	-5.53263	-0.98775
B	-0.01684	-1.88120	-3.98053
C	-0.33730	-0.36538	-3.46316
C	-1.26176	-2.60426	-4.73380
C	1.32332	-1.99525	-4.88734
H	0.37874	-0.09379	-2.64387
H	-0.14856	0.41319	-4.21268
H	-1.35975	-0.23066	-3.11952
H	-0.94846	-3.54330	-5.20509
H	-2.09543	-2.85801	-4.06759
H	-1.66860	-1.97316	-5.53406
H	1.65771	-3.03648	-4.96875
H	1.10630	-1.65986	-5.90918
H	2.17999	-1.40382	-4.54915
Cl	0.26450	-0.22926	2.17239
Na	-0.28349	-2.64276	2.05275

Calculated Structure **15**: Singlet

Mo	0.17268	-0.33056	-0.48307
P	-2.57088	-0.39950	-0.61760
P	2.72641	-0.39569	-0.72259
O	-0.67355	-2.83939	-2.17645
C	-1.32334	2.43872	0.02823
C	-0.58569	1.77719	-1.02732
C	0.83221	1.81508	-1.02815
C	1.50514	2.41916	0.10255
C	0.77854	3.02164	1.08195
C	-0.65041	3.05434	1.03483
C	-2.79672	2.38699	-0.00832
C	-3.47442	1.19378	-0.30626
C	-4.87398	1.21580	-0.35115
C	-5.59455	2.37475	-0.10492
C	-4.91723	3.55138	0.20304
C	-3.53352	3.55158	0.24802
C	2.97257	2.30881	0.19693
C	3.64105	1.10342	-0.09547
C	5.03193	1.07132	0.06705
C	5.75070	2.18482	0.48041
C	5.08433	3.37437	0.74883
C	3.70781	3.42671	0.60998
C	-3.60677	-1.51195	0.48636
C	-3.21588	-2.99734	0.34816
C	-3.59499	-0.99433	1.93310
C	-3.21058	-0.86084	-2.33808
C	-3.42027	0.36493	-3.23567
C	-4.45901	-1.74379	-2.42755
C	3.68562	-1.77486	0.10488
C	3.38237	-1.83869	1.60289
C	3.47945	-3.12734	-0.58150
C	3.40065	-0.48184	-2.49329
C	3.15657	0.79455	-3.30798
C	4.89462	-0.80886	-2.63214
C	-0.12270	-2.32076	-1.12040
C	0.14188	-2.78762	-0.04708
H	-1.08575	1.67101	-1.98269
H	1.36178	1.80727	-1.96762
H	1.28281	3.42260	1.95403
H	-1.19635	3.50837	1.85448
H	-5.42345	0.31273	-0.59036
H	-6.67713	2.36158	-0.16153
H	-5.46728	4.46687	0.38896
H	-2.99551	4.47061	0.45268
H	5.58614	0.16441	-0.13190
H	6.82802	2.12176	0.58362
H	5.63464	4.25614	1.05678
H	3.17787	4.35409	0.79722
H	-4.63184	-1.43011	0.12521
H	-2.66208	-3.21914	-0.56664
H	-4.11085	-3.62382	0.35529
H	-2.61541	-3.36598	1.18680
H	-2.63245	-0.55342	2.22575
H	-3.87371	-1.78578	2.63818
H	-4.31224	-0.18352	2.06290
H	-2.38758	-1.44841	-2.73540
H	-4.36490	0.86391	-3.00848
H	-3.45087	0.03990	-4.27948
H	-2.63486	1.11574	-3.15441
H	-4.35800	-2.69386	-1.90417
H	-4.62620	-1.98349	-3.48167
H	-5.36205	-1.24062	-2.07237
H	4.74156	-1.52395	0.00646
H	4.09850	-2.50435	2.09276
H	2.38345	-2.22972	1.80485
H	3.44234	-0.85752	2.07846
H	2.43541	-3.42984	-0.57751
H	4.05465	-3.89442	-0.05429
H	3.80642	-3.12630	-1.62189
H	2.81941	-1.29134	-2.94356
H	2.10639	0.98663	-3.50802
H	3.64475	0.68933	-4.28094
H	3.59518	1.66921	-2.81765
H	5.50663	0.06536	-2.39971
H	5.09332	-1.06820	-3.67571
H	5.24248	-1.64383	-2.02621
H	0.77089	-2.15967	0.62878
Si	-0.03940	-4.54901	0.50151
H	-0.49360	-4.52244	1.93887
H	-1.07899	-5.25742	-0.26614
H	1.22822	-5.31002	0.50608
B	-0.17997	-2.33904	-3.59401
C	0.00731	-0.71379	-3.48840
C	-1.29841	-2.76048	-4.69026
C	1.21664	-3.12860	-3.87057
H	0.60506	-0.39811	-2.59314
H	0.61256	-0.33442	-4.31905
H	-0.92353	-0.14561	-3.50560
H	-1.56390	-3.82023	-4.59549
H	-2.23633	-2.19079	-4.66337
H	-0.89544	-2.63297	-5.70250
H	1.02912	-4.18523	-4.09722
H	1.77078	-2.71805	-4.72494
H	1.89546	-3.11872	-3.00839
Cl	0.26879	-0.04584	2.27058
Na	-1.02635	-2.17368	2.24490

Calculated Structure **1**: Triplet

Mo	0.00143	-0.52208	-0.37640
P	-2.62502	-0.43559	-0.32922
P	2.72567	-0.39129	-0.41760
O	-0.17521	-0.64939	-3.44410
C	-1.38113	2.42486	0.38399
C	-0.60140	2.21775	-0.76049
C	0.78483	2.20083	-0.66626
C	1.41601	2.38214	0.56932
C	0.63853	2.65998	1.69096
C	-0.74990	2.68210	1.59782
C	-2.85529	2.36219	0.25051
C	-3.49401	1.20639	-0.22443
C	-4.88219	1.24182	-0.39988
C	-5.62546	2.37459	-0.10203
C	-4.98879	3.50252	0.40659
C	-3.61312	3.49165	0.57684
C	2.89184	2.28152	0.63634
C	3.59131	1.17356	0.11861
C	4.99208	1.21449	0.14583
C	5.68576	2.29249	0.67740
C	4.98506	3.36208	1.22254
C	3.59999	3.35022	1.19738
C	-3.61173	-1.25360	1.04485
C	-3.08587	-2.65057	1.35527
C	-3.60426	-0.40324	2.31987
C	-3.24567	-1.19247	-1.93760
C	-3.35198	-0.12025	-3.02620
C	-4.50602	-2.05625	-1.89197
C	3.76538	-1.61094	0.56087
C	3.60798	-1.39053	2.06500
C	3.50500	-3.06952	0.18346
C	3.31176	-0.68578	-2.17891
C	2.97433	0.50718	-3.07637
C	4.77514	-1.07497	-2.40377
C	-0.09767	-0.56961	-2.28323
C	0.21240	-2.56982	-0.70277
H	-1.08340	2.11550	-1.72607
H	1.38568	2.09403	-1.56030
H	1.11567	2.77680	2.65738
H	-1.34905	2.82446	2.49058
H	-5.40130	0.35828	-0.75154
H	-6.69931	2.37109	-0.25024
H	-5.56079	4.38827	0.65820
H	-3.10114	4.37283	0.94893
H	5.56720	0.38115	-0.23580
H	6.76978	2.28904	0.67638
H	5.51445	4.20466	1.65238
H	3.04154	4.19277	1.59113
H	-4.64014	-1.33585	0.67756
H	-2.10524	-2.56117	1.82935
H	-2.99800	-3.28592	0.47520
H	-3.74645	-3.15278	2.06740
H	-2.58110	-0.19923	2.64268
H	-4.10469	-0.95479	3.12152
H	-4.12816	0.54463	2.19132
H	-2.41322	-1.84710	-2.20900
H	-4.23540	0.50613	-2.88877
H	-3.42658	-0.59937	-4.00560
H	-2.47684	0.53098	-3.05176
H	-4.44904	-2.84730	-1.14323
H	-4.62986	-2.54333	-2.86369
H	-5.41299	-1.47578	-1.70718
H	4.80394	-1.39354	0.30312
H	4.23008	-2.10624	2.61076
H	2.57181	-1.50919	2.38686
H	3.91309	-0.38518	2.36250
H	2.52123	-3.40113	0.51742
H	4.25764	-3.70721	0.65594
H	3.54207	-3.24969	-0.89354
H	2.67781	-1.52414	-2.49005
H	1.90898	0.72698	-3.09485
H	3.27220	0.28543	-4.10482
H	3.52044	1.40098	-2.75833
H	5.43790	-0.21495	-2.28573
H	4.89006	-1.42181	-3.43465
H	5.12704	-1.87801	-1.75546
H	1.17473	-2.76966	-1.19221
Si	-0.77337	-4.08559	-0.96759
H	-1.02548	-4.81674	0.34159
H	-2.16024	-3.97219	-1.51183
H	-0.06334	-5.09266	-1.80397
B	0.09720	-2.49675	-5.16395
C	0.19805	-1.45199	-6.33918
C	-1.29534	-3.14032	-4.79934
C	1.41397	-3.07297	-4.51336
H	0.91094	-0.65500	-6.10850
H	0.59422	-1.96200	-7.22827
H	-0.75311	-0.99546	-6.62329
H	-1.29710	-3.73692	-3.88404
H	-2.08173	-2.38297	-4.72711
H	-1.59737	-3.80680	-5.61955
H	1.29515	-3.21705	-3.43465
H	1.59565	-4.07482	-4.92681
H	2.31212	-2.47674	-4.70151
Cl	0.06052	-0.54037	2.38140
Na	0.25316	-2.98255	1.71546

Calculated Structure **2**: Triplet

Mo	-0.00359	-0.50956	-0.37966
P	-2.62970	-0.42114	-0.33200
P	2.71889	-0.38204	-0.42253
O	-0.18132	-0.64952	-3.44685
C	-1.38694	2.43723	0.38173
C	-0.60318	2.23056	-0.76001
C	0.78262	2.21050	-0.66016
C	1.40944	2.38737	0.57852
C	0.62789	2.66420	1.69762
C	-0.76011	2.69001	1.59858
C	-2.86050	2.37709	0.24193
C	-3.49850	1.22114	-0.23360
C	-4.88600	1.25721	-0.41404
C	-5.62919	2.39163	-0.12190
C	-4.99320	3.52010	0.38624
C	-3.61827	3.50802	0.56242
C	2.88496	2.28339	0.65048
C	3.58493	1.17868	0.12552
C	4.98574	1.21836	0.15662
C	5.67884	2.29116	0.69934
C	4.97773	3.35647	1.25207
C	3.59279	3.34647	1.22271
C	-3.61591	-1.23457	1.04464
C	-3.09064	-2.63162	1.35563
C	-3.60460	-0.38149	2.31772
C	-3.24977	-1.18505	-1.93685
C	-3.35165	-0.11842	-3.03150
C	-4.51207	-2.04585	-1.88934
C	3.75920	-1.60933	0.54569
C	3.60178	-1.40126	2.05163
C	3.50033	-3.06483	0.15546
C	3.30380	-0.66419	-2.18586
C	2.96132	0.53262	-3.07631
C	4.76853	-1.04625	-2.41408
C	-0.10408	-0.56239	-2.28650
C	0.20822	-2.55593	-0.71566
H	-1.08139	2.13119	-1.72774
H	1.38708	2.10475	-1.55187
H	1.10126	2.77692	2.66637
H	-1.36243	2.83193	2.48920
H	-5.40457	0.37322	-0.76538
H	-6.70244	2.38901	-0.27436
H	-5.56518	4.40716	0.63313
H	-3.10710	4.38950	0.93469
H	5.56117	0.38797	-0.23095
H	6.76281	2.28681	0.70107
H	5.50664	4.19474	1.69070
H	3.03411	4.18645	1.62154
H	-4.64505	-1.31557	0.67894
H	-2.10712	-2.54301	1.82382
H	-3.00842	-3.26887	0.47626
H	-3.74820	-3.13150	2.07216
H	-2.58041	-0.18032	2.63911
H	-4.10619	-0.92934	3.12112
H	-4.12545	0.56784	2.18712
H	-2.41809	-1.84324	-2.20192
H	-4.23805	0.50563	-2.90254
H	-3.41829	-0.60191	-4.00943
H	-2.47879	0.53585	-3.05421
H	-4.45850	-2.83290	-1.13620
H	-4.63493	-2.53796	-2.85861
H	-5.41816	-1.46244	-1.70960
H	4.79766	-1.38889	0.29027
H	4.22350	-2.12150	2.59182
H	2.56554	-1.52125	2.37287
H	3.90706	-0.39835	2.35723
H	2.51537	-3.39956	0.48262
H	4.25177	-3.70617	0.62493
H	3.54125	-3.23569	-0.92290
H	2.67249	-1.50311	-2.50091
H	1.89507	0.74825	-3.09341
H	3.26014	0.31854	-4.10609
H	3.50392	1.42674	-2.75289
H	5.42770	-0.18415	-2.29081
H	4.88429	-1.38619	-3.44716
H	5.12411	-1.85181	-1.77092
H	1.16258	-2.75339	-1.22103
Si	-0.77980	-4.07275	-0.96401
H	-1.03589	-4.78474	0.35552
H	-2.16501	-3.97062	-1.51508
H	-0.06457	-5.09186	-1.78111
B	0.08519	-2.50912	-5.16407
C	0.13681	-1.46421	-6.34252
C	-1.28680	-3.18471	-4.77870
C	1.42781	-3.04988	-4.53717
H	0.84617	-0.65700	-6.13924
H	0.50724	-1.97282	-7.24358
H	-0.82985	-1.02202	-6.59583
H	-1.24937	-3.83541	-3.90210
H	-2.06496	-2.43101	-4.62176
H	-1.63261	-3.79463	-5.62474
H	1.32267	-3.25112	-3.46636
H	1.65401	-4.02072	-5.00061
H	2.29640	-2.40512	-4.70223
Cl	0.05830	-0.53564	2.37591
Na	0.25704	-2.97586	1.70419

Calculated Structure **3**: Triplet

Mo	0.01630	-0.48634	-0.38586
P	-2.60447	-0.39487	-0.34368
P	2.73485	-0.36992	-0.42696
O	-0.11962	-0.77386	-3.44214
C	-1.36077	2.44705	0.38637
C	-0.56329	2.24547	-0.74760
C	0.82122	2.22348	-0.62963
C	1.43314	2.38433	0.61859
C	0.63837	2.65232	1.73025
C	-0.74813	2.68586	1.61326
C	-2.83296	2.39817	0.22589
C	-3.47110	1.24680	-0.26103
C	-4.85498	1.29038	-0.46289
C	-5.59544	2.42980	-0.18154
C	-4.96053	3.55370	0.33779
C	-3.58830	3.53341	0.53590
C	2.90657	2.26912	0.70736
C	3.60567	1.17102	0.16719
C	5.00597	1.19933	0.21826
C	5.69961	2.25443	0.79432
C	4.99877	3.31283	1.36067
C	3.61420	3.31395	1.31207
C	-3.58852	-1.20446	1.03395
C	-3.06270	-2.60367	1.33764
C	-3.57629	-0.35322	2.30774
C	-3.22016	-1.18105	-1.93600
C	-3.28003	-0.14097	-3.05842
C	-4.49471	-2.02379	-1.89447
C	3.76834	-1.63323	0.50133
C	3.60552	-1.48173	2.01339
C	3.51042	-3.07263	0.05431
C	3.31915	-0.60565	-2.19654
C	2.94886	0.59818	-3.06571
C	4.79111	-0.95192	-2.43189
C	-0.06611	-0.63061	-2.28495
C	0.23723	-2.51407	-0.82874
H	-1.02922	2.15560	-1.72250
H	1.43602	2.12680	-1.51491
H	1.09884	2.75258	2.70635
H	-1.36155	2.82404	2.49689
H	-5.37282	0.40969	-0.82314
H	-6.66614	2.43432	-0.35110
H	-5.53083	4.44413	0.57641
H	-3.07764	4.41144	0.91709
H	5.58106	0.37385	-0.18037
H	6.78344	2.24152	0.81083
H	5.52771	4.13724	1.82492
H	3.05669	4.14951	1.72149
H	-4.61813	-1.28219	0.66851
H	-2.08922	-2.51661	1.82667
H	-2.96116	-3.22956	0.45125
H	-3.73132	-3.11633	2.03463
H	-2.55215	-0.15801	2.63291
H	-4.08393	-0.89809	3.10928
H	-4.09154	0.59909	2.17430
H	-2.39487	-1.85816	-2.16700
H	-4.16600	0.49138	-2.97039
H	-3.31711	-0.64859	-4.02626
H	-2.40181	0.50684	-3.06843
H	-4.46424	-2.79845	-1.12722
H	-4.60777	-2.53128	-2.85709
H	-5.39635	-1.42656	-1.74077
H	4.80825	-1.40520	0.25946
H	4.23480	-2.21371	2.52830
H	2.57074	-1.62548	2.32865
H	3.89734	-0.48693	2.35606
H	2.51795	-3.41506	0.34889
H	4.25099	-3.73367	0.51361
H	3.57177	-3.20348	-1.02881
H	2.70475	-1.45188	-2.52622
H	1.87711	0.78753	-3.07928
H	3.25224	0.40899	-4.09907
H	3.47091	1.49920	-2.72737
H	5.43201	-0.08018	-2.28210
H	4.91606	-1.26100	-3.47361
H	5.16088	-1.76791	-1.81012
H	1.17780	-2.70312	-1.36052
Si	-0.73911	-4.04175	-1.04657
H	-0.99188	-4.72079	0.29469
H	-2.12673	-3.98187	-1.59964
H	0.00014	-5.07450	-1.82271
B	0.13720	-2.68952	-5.17491
C	0.04120	-1.62627	-6.33209
C	-1.16152	-3.47573	-4.74514
C	1.53787	-3.10209	-4.58112
H	0.78987	-0.83405	-6.25638
H	0.22616	-2.14512	-7.28390
H	-0.94760	-1.16734	-6.41697
H	-0.97917	-4.40030	-4.19202
H	-1.74138	-2.81583	-4.08645
H	-1.81643	-3.69567	-5.59502
H	1.47024	-3.40218	-3.53057
H	1.88212	-3.99377	-5.12486
H	2.31452	-2.33997	-4.69302
Cl	0.09181	-0.57295	2.35723
Na	0.27467	-2.99465	1.59677

Calculated Structure **4**: Triplet

Mo	0.01410	-0.47673	-0.37004
P	-2.60732	-0.39423	-0.34328
P	2.72877	-0.36179	-0.43204
O	-0.11099	-0.85793	-3.41522
C	-1.36177	2.44543	0.39842
C	-0.56873	2.24435	-0.73910
C	0.81631	2.22875	-0.62793
C	1.43360	2.39212	0.61712
C	0.64342	2.65806	1.73284
C	-0.74393	2.68751	1.62239
C	-2.83471	2.39494	0.24429
C	-3.47426	1.24651	-0.24834
C	-4.85862	1.29161	-0.44698
C	-5.59850	2.42847	-0.15476
C	-4.96246	3.54839	0.37147
C	-3.58973	3.52744	0.56498
C	2.90741	2.27873	0.69842
C	3.60428	1.18058	0.15470
C	5.00492	1.21003	0.19958
C	5.70036	2.26562	0.77253
C	5.00163	3.32364	1.34192
C	3.61693	3.32399	1.29985
C	-3.59323	-1.21823	1.02290
C	-3.06844	-2.62141	1.30819
C	-3.57891	-0.38255	2.30655
C	-3.21654	-1.16878	-1.94372
C	-3.25569	-0.12157	-3.06021
C	-4.50027	-1.99833	-1.91655
C	3.76790	-1.62378	0.49208
C	3.60930	-1.47068	2.00439
C	3.51332	-3.06438	0.04728
C	3.29917	-0.60152	-2.20586
C	2.91016	0.59418	-3.07806
C	4.77253	-0.93526	-2.45120
C	-0.06171	-0.69574	-2.25881
C	0.24632	-2.49649	-0.86152
H	-1.03855	2.15122	-1.71160
H	1.42713	2.13320	-1.51588
H	1.10844	2.76007	2.70674
H	-1.35352	2.82442	2.50896
H	-5.37723	0.41373	-0.81284
H	-6.66964	2.43396	-0.32127
H	-5.53246	4.43654	0.61893
H	-3.07835	4.40303	0.95079
H	5.57908	0.38506	-0.20134
H	6.78425	2.25328	0.78440
H	5.53232	4.14825	1.80380
H	3.06066	4.15899	1.71217
H	-4.62296	-1.29043	0.65671
H	-2.09320	-2.54227	1.79532
H	-2.97025	-3.23665	0.41403
H	-3.73545	-3.14186	2.00096
H	-2.55426	-0.19357	2.63414
H	-4.08798	-0.93569	3.10156
H	-4.09177	0.57262	2.18452
H	-2.39725	-1.85354	-2.17347
H	-4.12646	0.53088	-2.96612
H	-3.30691	-0.62228	-4.03085
H	-2.36167	0.50422	-3.06848
H	-4.48416	-2.77637	-1.15220
H	-4.61046	-2.50081	-2.88202
H	-5.39718	-1.39272	-1.76833
H	4.80666	-1.39397	0.24714
H	4.23950	-2.20243	2.51854
H	2.57529	-1.61283	2.32325
H	3.90327	-0.47562	2.34489
H	2.52215	-3.41000	0.34278
H	4.25587	-3.72250	0.50761
H	3.57496	-3.19710	-1.03550
H	2.69068	-1.45507	-2.52774
H	1.83684	0.77460	-3.08064
H	3.20359	0.40043	-4.11337
H	3.42938	1.50107	-2.75131
H	5.40608	-0.05644	-2.31219
H	4.89244	-1.25015	-3.49169
H	5.15514	-1.74355	-1.82695
H	1.19194	-2.69156	-1.37984
Si	-0.72717	-4.02656	-1.06940
H	-0.98017	-4.70139	0.27471
H	-2.11396	-3.97443	-1.62437
H	0.01845	-5.06022	-1.83767
B	0.15070	-2.70577	-5.16750
C	0.07633	-1.61814	-6.30402
C	-1.16023	-3.48841	-4.76660
C	1.54534	-3.15236	-4.58326
H	0.80107	-0.81137	-6.16911
H	0.32600	-2.10559	-7.25753
H	-0.91747	-1.17940	-6.42716
H	-0.99870	-4.38618	-4.16554
H	-1.79632	-2.81112	-4.18238
H	-1.75238	-3.76081	-5.64774
H	1.47404	-3.43269	-3.52764
H	1.85928	-4.06340	-5.11270
H	2.34375	-2.41506	-4.70925
Cl	0.08840	-0.58001	2.37148
Na	0.28026	-2.99178	1.57111

Calculated Structure **5**: Triplet

Mo	0.00792	-0.47187	-0.35280
P	-2.61172	-0.39143	-0.34682
P	2.72395	-0.36257	-0.42136
O	-0.09435	-0.90552	-3.39505
C	-1.35967	2.44196	0.40829
C	-0.56705	2.24222	-0.72982
C	0.81802	2.22871	-0.61930
C	1.43609	2.39159	0.62525
C	0.64626	2.65492	1.74200
C	-0.74112	2.68347	1.63234
C	-2.83269	2.39486	0.25412
C	-3.47535	1.24999	-0.24226
C	-4.85932	1.29972	-0.44222
C	-5.59595	2.43823	-0.14805
C	-4.95689	3.55497	0.38134
C	-3.58446	3.52916	0.57652
C	2.91003	2.27796	0.70477
C	3.60436	1.17774	0.16228
C	5.00501	1.20470	0.20519
C	5.70285	2.26072	0.77451
C	5.00659	3.32142	1.34205
C	3.62173	3.32377	1.30236
C	-3.60330	-1.22916	1.00639
C	-3.08033	-2.63616	1.27671
C	-3.59327	-0.40797	2.29931
C	-3.21394	-1.15041	-1.95694
C	-3.23232	-0.09513	-3.06588
C	-4.50426	-1.96988	-1.94667
C	3.76158	-1.62782	0.50062
C	3.60258	-1.47699	2.01315
C	3.50541	-3.06722	0.05286
C	3.28903	-0.60389	-2.19652
C	2.89148	0.58725	-3.07107
C	4.76310	-0.93206	-2.44472
C	-0.05395	-0.75125	-2.23426
C	0.24475	-2.48214	-0.90957
H	-1.03669	2.14905	-1.70249
H	1.42801	2.13298	-1.50777
H	1.11188	2.75698	2.71561
H	-1.35036	2.81982	2.51922
H	-5.38011	0.42454	-0.81118
H	-6.66685	2.44763	-0.31592
H	-5.52427	4.44457	0.62966
H	-3.07072	4.40254	0.96426
H	5.57724	0.37792	-0.19481
H	6.78676	2.24681	0.78478
H	5.53939	4.14649	1.80067
H	3.06725	4.16058	1.71347
H	-4.63171	-1.29654	0.63569
H	-2.10751	-2.56397	1.77004
H	-2.97781	-3.24016	0.37518
H	-3.75088	-3.16509	1.95953
H	-2.56996	-0.22677	2.63529
H	-4.10958	-0.96763	3.08503
H	-4.10141	0.55062	2.18444
H	-2.39909	-1.84054	-2.18588
H	-4.09038	0.57353	-2.96836
H	-3.29158	-0.58847	-4.03982
H	-2.32512	0.51160	-3.06873
H	-4.50100	-2.75295	-1.18714
H	-4.60918	-2.46551	-2.91626
H	-5.39807	-1.35874	-1.80322
H	4.80083	-1.39962	0.25632
H	4.23357	-2.20872	2.52635
H	2.56884	-1.62093	2.33208
H	3.89585	-0.48214	2.35478
H	2.51174	-3.41141	0.34187
H	4.24311	-3.72811	0.51693
H	3.57308	-3.19884	-1.02969
H	2.68350	-1.46059	-2.51531
H	1.81699	0.76126	-3.07126
H	3.18298	0.39123	-4.10653
H	3.40753	1.49773	-2.74915
H	5.39327	-0.05020	-2.30966
H	4.88170	-1.24948	-3.48459
H	5.15073	-1.73705	-1.81914
H	1.20082	-2.68272	-1.40430
Si	-0.72914	-4.01072	-1.12277
H	-0.98068	-4.69625	0.21656
H	-2.11612	-3.95287	-1.67508
H	0.01658	-5.03835	-1.89834
B	0.18048	-2.68676	-5.17183
C	0.12031	-1.57536	-6.28644
C	-1.13698	-3.47734	-4.80697
C	1.56961	-3.15631	-4.59140
H	0.85413	-0.77968	-6.13569
H	0.36290	-2.04646	-7.24992
H	-0.86844	-1.12260	-6.39937
H	-0.98480	-4.38645	-4.22062
H	-1.78626	-2.81281	-4.22277
H	-1.71070	-3.73535	-5.70462
H	1.49194	-3.46889	-3.54533
H	1.88488	-4.05107	-5.14713
H	2.37064	-2.41765	-4.69016
Cl	0.07793	-0.59943	2.38587
Na	0.27031	-2.99590	1.52934

Calculated Structure **6**: Triplet

Mo	0.01479	-0.46100	-0.33955
P	-2.61111	-0.39477	-0.33217
P	2.72119	-0.36503	-0.43150
O	-0.10186	-0.96443	-3.37642
C	-1.36128	2.43990	0.40442
C	-0.57745	2.22472	-0.73753
C	0.80867	2.21032	-0.63723
C	1.43621	2.39137	0.60110
C	0.65471	2.66789	1.72026
C	-0.73366	2.69520	1.62084
C	-2.83509	2.39148	0.26239
C	-3.47970	1.24390	-0.22464
C	-4.86528	1.29066	-0.41372
C	-5.60121	2.42901	-0.11777
C	-4.95972	3.54866	0.40223
C	-3.58582	3.52587	0.58661
C	2.91081	2.28241	0.67161
C	3.60426	1.18011	0.13287
C	5.00496	1.20960	0.16751
C	5.70400	2.27079	0.72537
C	5.00893	3.33417	1.28929
C	3.62385	3.33390	1.25754
C	-3.59501	-1.23607	1.02389
C	-3.06923	-2.64295	1.28936
C	-3.57836	-0.41657	2.31766
C	-3.21631	-1.15471	-1.94068
C	-3.22818	-0.10088	-3.05079
C	-4.51041	-1.96826	-1.92878
C	3.76517	-1.62013	0.49723
C	3.61755	-1.45296	2.00922
C	3.50815	-3.06498	0.06788
C	3.27425	-0.62291	-2.20778
C	2.86196	0.55623	-3.09186
C	4.74844	-0.94555	-2.46247
C	-0.05186	-0.82550	-2.20929
C	0.24883	-2.47372	-0.94321
H	-1.05413	2.12134	-1.70580
H	1.41171	2.10701	-1.52961
H	1.12766	2.78159	2.68903
H	-1.33622	2.84158	2.51066
H	-5.38759	0.41358	-0.77558
H	-6.67338	2.43613	-0.27699
H	-5.52645	4.43831	0.65161
H	-3.07041	4.40163	0.96662
H	5.57631	0.38090	-0.22964
H	6.78791	2.25893	0.72978
H	5.54279	4.16341	1.73899
H	3.07037	4.17273	1.66586
H	-4.62522	-1.30405	0.65861
H	-2.09647	-2.57020	1.78299
H	-2.96630	-3.24427	0.38596
H	-3.73778	-3.17525	1.97142
H	-2.55305	-0.23260	2.64641
H	-4.08739	-0.97847	3.10652
H	-4.08997	0.54073	2.20735
H	-2.40559	-1.84917	-2.17064
H	-4.07223	0.58414	-2.94462
H	-3.30794	-0.59426	-4.02313
H	-2.30833	0.48642	-3.06525
H	-4.51112	-2.74896	-1.16665
H	-4.61658	-2.46660	-2.89677
H	-5.40176	-1.35304	-1.78843
H	4.80235	-1.39408	0.24253
H	4.25698	-2.17521	2.52536
H	2.58737	-1.59957	2.33850
H	3.90781	-0.45267	2.33727
H	2.51804	-3.40867	0.36997
H	4.25025	-3.71908	0.53437
H	3.56782	-3.20953	-1.01337
H	2.67182	-1.48608	-2.51393
H	1.78595	0.72113	-3.08627
H	3.14748	0.35095	-4.12716
H	3.37398	1.47384	-2.78377
H	5.37490	-0.05928	-2.33957
H	4.86198	-1.27209	-3.50003
H	5.14421	-1.74284	-1.83201
H	1.22041	-2.68875	-1.39812
Si	-0.72021	-4.00778	-1.13329
H	-0.95363	-4.68899	0.21239
H	-2.11256	-3.95237	-1.66894
H	0.01910	-5.03798	-1.91073
B	0.16015	-2.66193	-5.15309
C	0.10496	-1.53743	-6.25597
C	-1.16120	-3.45746	-4.80887
C	1.55071	-3.16196	-4.60004
H	0.84181	-0.74690	-6.09266
H	0.34760	-1.99607	-7.22528
H	-0.88129	-1.07779	-6.36326
H	-1.02144	-4.33824	-4.17807
H	-1.86204	-2.78610	-4.29815
H	-1.67181	-3.77368	-5.72669
H	1.48249	-3.48974	-3.55793
H	1.84687	-4.05132	-5.17445
H	2.36045	-2.43238	-4.69729
Cl	0.09385	-0.59156	2.40360
Na	0.27249	-2.97841	1.51087

Calculated Structure **7**: Triplet

Mo	0.04057	-0.60579	-0.30861
P	-2.68381	-0.45671	-0.31065
P	2.70820	-0.52114	-0.18668
O	0.36341	-1.96649	-3.08750
C	-1.32573	2.42192	0.12191
C	-0.67083	1.97558	-1.03562
C	0.71653	1.95689	-1.09698
C	1.47518	2.39608	-0.00211
C	0.82358	2.88909	1.12287
C	-0.56825	2.89981	1.18608
C	-2.80407	2.37515	0.16031
C	-3.50476	1.20333	-0.15919
C	-4.90334	1.25506	-0.20397
C	-5.59734	2.42040	0.08203
C	-4.89609	3.56850	0.44086
C	-3.51159	3.54173	0.47476
C	2.95046	2.31920	-0.09076
C	3.59924	1.10048	-0.34093
C	4.99131	1.10801	-0.48110
C	5.72737	2.27876	-0.36761
C	5.07918	3.47672	-0.08440
C	3.69967	3.49145	0.05045
C	-3.66086	-1.30106	1.06128
C	-3.11044	-2.68514	1.41164
C	-3.72746	-0.45109	2.33615
C	-3.39116	-1.12792	-1.92940
C	-3.79229	-0.02548	-2.91760
C	-4.51981	-2.15177	-1.80767
C	3.60584	-1.09237	1.35978
C	3.55630	-0.03809	2.47033
C	3.07575	-2.42707	1.88582
C	3.40490	-1.58838	-1.56616
C	3.45736	-0.78152	-2.86512
C	4.70770	-2.35309	-1.32242
C	0.20902	-1.47969	-1.98729
C	0.22729	-2.75912	-0.45017
H	-1.24408	1.69530	-1.91172
H	1.21207	1.65741	-2.01371
H	1.40673	3.20888	1.97978
H	-1.06546	3.22118	2.09460
H	-5.46615	0.35860	-0.44227
H	-6.68037	2.43064	0.03772
H	-5.42759	4.48309	0.67731
H	-2.95496	4.44049	0.71819
H	5.51958	0.18052	-0.65991
H	6.80455	2.25290	-0.48587
H	5.64530	4.39523	0.01901
H	3.17921	4.42306	0.24573
H	-4.67345	-1.42649	0.66925
H	-2.30751	-2.55974	2.14331
H	-2.74213	-3.24955	0.55481
H	-3.88432	-3.28222	1.90091
H	-2.72641	-0.16757	2.66682
H	-4.19160	-1.04174	3.13221
H	-4.31834	0.45492	2.20731
H	-2.52298	-1.63869	-2.34775
H	-4.79293	0.35661	-2.70758
H	-3.79088	-0.43661	-3.93029
H	-3.11402	0.82791	-2.91369
H	-4.28098	-2.97591	-1.13416
H	-4.70754	-2.58472	-2.79439
H	-5.45515	-1.69414	-1.47287
H	4.64839	-1.22563	1.05352
H	4.01633	-0.44600	3.37552
H	2.52467	0.22779	2.71042
H	4.10036	0.86802	2.20045
H	2.15331	-2.23846	2.44158
H	3.79067	-2.85911	2.59118
H	2.88849	-3.16423	1.10186
H	2.62117	-2.33687	-1.70233
H	2.51340	-0.26650	-3.05938
H	3.62658	-1.45642	-3.70652
H	4.25936	-0.04022	-2.84954
H	5.58473	-1.70658	-1.25947
H	4.87545	-3.02723	-2.16671
H	4.67542	-2.96749	-0.42063
H	1.27501	-3.08946	-0.44267
Si	-0.75679	-4.13174	-1.17176
H	-0.07733	-4.85706	-2.27672
H	-1.07503	-5.18453	-0.14736
H	-2.08325	-3.68695	-1.67297
B	-0.08755	-1.33392	-4.67348
C	-0.40904	0.21464	-4.39139
C	-1.34674	-2.26498	-5.03467
C	1.21308	-1.62654	-5.56537
H	-1.19479	0.34209	-3.64113
H	0.46986	0.78331	-4.06125
H	-0.76634	0.69652	-5.30915
H	-1.07634	-3.32579	-5.07573
H	-2.19018	-2.17389	-4.34061
H	-1.72902	-1.99701	-6.02778
H	1.58560	-2.64862	-5.43249
H	0.95139	-1.52716	-6.62619
H	2.04483	-0.93829	-5.38531
Cl	-0.08720	-0.33529	2.41367
Na	-0.07091	-2.85781	1.92966

Calculated Structure **8**: Triplet

Mo	0.04110	-0.58967	-0.31571
P	-2.67875	-0.44197	-0.32378
P	2.71211	-0.51780	-0.19185
O	0.32777	-2.03577	-3.07796
C	-1.32141	2.43428	0.10745
C	-0.65656	1.98512	-1.04402
C	0.73123	1.96146	-1.09099
C	1.48095	2.39963	0.01123
C	0.81989	2.89322	1.12965
C	-0.57312	2.90764	1.17907
C	-2.80009	2.39167	0.12978
C	-3.49916	1.21933	-0.19059
C	-4.89704	1.27207	-0.24920
C	-5.59202	2.44036	0.02211
C	-4.89269	3.58986	0.38032
C	-3.50858	3.56125	0.42949
C	2.95667	2.32143	-0.06634
C	3.60625	1.10433	-0.32277
C	4.99930	1.11217	-0.45253
C	5.73537	2.28132	-0.32405
C	5.08609	3.47736	-0.03548
C	3.70566	3.49192	0.08997
C	-3.65704	-1.26919	1.05886
C	-3.10750	-2.64877	1.42973
C	-3.73087	-0.40416	2.32315
C	-3.38583	-1.13365	-1.93400
C	-3.79487	-0.04561	-2.93574
C	-4.50899	-2.16206	-1.79909
C	3.60478	-1.11098	1.34887
C	3.54804	-0.07646	2.47718
C	3.07905	-2.45708	1.84798
C	3.40985	-1.57052	-1.58070
C	3.43962	-0.75320	-2.87325
C	4.72438	-2.32113	-1.35661
C	0.20313	-1.55809	-1.95655
C	0.24339	-2.76262	-0.48772
H	-1.22154	1.71004	-1.92725
H	1.23495	1.66164	-2.00344
H	1.39526	3.21172	1.99214
H	-1.07819	3.23105	2.08239
H	-5.45851	0.37471	-0.48703
H	-6.67451	2.45215	-0.03341
H	-5.42524	4.50689	0.60465
H	-2.95319	4.46064	0.67334
H	5.52840	0.18599	-0.63487
H	6.81333	2.25559	-0.43489
H	5.65204	4.39464	0.07920
H	3.18467	4.42247	0.28871
H	-4.66800	-1.39996	0.66443
H	-2.31809	-2.51341	2.17476
H	-2.72625	-3.21871	0.58202
H	-3.88679	-3.24587	1.91023
H	-2.73141	-0.12421	2.66126
H	-4.20656	-0.98332	3.12085
H	-4.31509	0.50369	2.17847
H	-2.51536	-1.64443	-2.34810
H	-4.80497	0.31910	-2.74047
H	-3.77332	-0.46509	-3.94473
H	-3.13281	0.82036	-2.93154
H	-4.26707	-2.97610	-1.11442
H	-4.69338	-2.60883	-2.78026
H	-5.44701	-1.70490	-1.47128
H	4.64892	-1.23490	1.04402
H	4.01281	-0.49611	3.37452
H	2.51504	0.17771	2.72307
H	4.08495	0.83814	2.22180
H	2.14082	-2.28706	2.38271
H	3.78261	-2.88785	2.56543
H	2.92069	-3.18748	1.05157
H	2.63375	-2.32751	-1.71493
H	2.47960	-0.26732	-3.06387
H	3.62991	-1.41570	-3.71981
H	4.21922	0.01180	-2.85067
H	5.59546	-1.66524	-1.31368
H	4.88325	-2.99616	-2.20192
H	4.71573	-2.93322	-0.45279
H	1.28801	-3.09771	-0.45416
Si	-0.76602	-4.16000	-1.12235
H	-0.09720	-4.96192	-2.17742
H	-1.09492	-5.14097	-0.02943
H	-2.08578	-3.71965	-1.64156
B	-0.08537	-1.36300	-4.59480
C	-0.40910	0.18779	-4.30462
C	-1.35351	-2.26455	-5.02040
C	1.20630	-1.62961	-5.51737
H	-1.19935	0.30896	-3.55827
H	0.46650	0.75579	-3.96353
H	-0.76029	0.67643	-5.22100
H	-1.08648	-3.32257	-5.12267
H	-2.19866	-2.21534	-4.32330
H	-1.73328	-1.93804	-5.99660
H	1.59869	-2.64607	-5.39496
H	0.92432	-1.53154	-6.57293
H	2.03144	-0.92955	-5.35203
Cl	-0.09138	-0.36506	2.41300
Na	-0.10186	-2.87906	1.88991

Calculated Structure **9**: Triplet

Mo	0.04696	-0.57946	-0.33160
P	-2.67340	-0.42993	-0.33397
P	2.72107	-0.50924	-0.20208
O	0.30760	-2.09220	-3.07751
C	-1.32316	2.44528	0.09381
C	-0.64750	1.99951	-1.05313
C	0.74049	1.97270	-1.08504
C	1.47974	2.40504	0.02723
C	0.80811	2.89329	1.14110
C	-0.58582	2.90983	1.17602
C	-2.80196	2.40511	0.09956
C	-3.49719	1.23163	-0.22520
C	-4.89469	1.28249	-0.29379
C	-5.59235	2.45112	-0.03058
C	-4.89693	3.60220	0.32972
C	-3.51325	3.57499	0.39047
C	2.95630	2.32988	-0.03606
C	3.61211	1.11744	-0.29967
C	5.00667	1.13118	-0.41344
C	5.73764	2.30096	-0.26428
C	5.08179	3.49171	0.03031
C	3.70025	3.50067	0.14143
C	-3.64444	-1.22650	1.07292
C	-3.09586	-2.59898	1.47335
C	-3.71616	-0.33457	2.31862
C	-3.38983	-1.15918	-1.92324
C	-3.81844	-0.09718	-2.94565
C	-4.50132	-2.19592	-1.75673
C	3.61040	-1.13163	1.32876
C	3.54088	-0.12645	2.48223
C	3.09597	-2.49546	1.78820
C	3.42475	-1.53527	-1.60722
C	3.42653	-0.70002	-2.88821
C	4.75554	-2.26395	-1.40799
C	0.20650	-1.63134	-1.93445
C	0.27348	-2.76660	-0.53920
H	-1.20455	1.73187	-1.94392
H	1.25399	1.67759	-1.99384
H	1.37489	3.20688	2.01096
H	-1.09990	3.23050	2.07525
H	-5.45348	0.38366	-0.53167
H	-6.67436	2.46167	-0.09356
H	-5.43199	4.51927	0.54753
H	-2.96026	4.47491	0.63762
H	5.54086	0.20877	-0.59917
H	6.81675	2.27935	-0.36366
H	5.64350	4.40936	0.16108
H	3.17435	4.42739	0.34492
H	-4.65667	-1.36352	0.68408
H	-2.32074	-2.44907	2.23101
H	-2.70175	-3.17925	0.63804
H	-3.88035	-3.19416	1.94754
H	-2.71602	-0.05598	2.65554
H	-4.19890	-0.89393	3.12615
H	-4.29395	0.57389	2.15307
H	-2.51719	-1.66955	-2.33451
H	-4.83877	0.24503	-2.76323
H	-3.77902	-0.53312	-3.94705
H	-3.17799	0.78489	-2.95233
H	-4.24621	-2.99317	-1.05719
H	-4.68935	-2.66459	-2.72691
H	-5.44107	-1.74143	-1.43038
H	4.65696	-1.23781	1.02532
H	4.02007	-0.55870	3.36588
H	2.50539	0.10232	2.74064
H	4.05884	0.80407	2.24556
H	2.13658	-2.35595	2.29277
H	3.78500	-2.92446	2.52065
H	2.97909	-3.21412	0.97440
H	2.66075	-2.30455	-1.74319
H	2.44994	-0.24495	-3.07083
H	3.63791	-1.34317	-3.74454
H	4.18112	0.08964	-2.85417
H	5.61538	-1.59261	-1.38467
H	4.90866	-2.93631	-2.25643
H	4.77644	-2.87600	-0.50446
H	1.31475	-3.10518	-0.47724
Si	-0.76416	-4.19276	-1.05297
H	-0.11829	-5.09139	-2.03991
H	-1.08794	-5.07301	0.12840
H	-2.08514	-3.77266	-1.58294
B	-0.10003	-1.38446	-4.53638
C	-0.44324	0.16097	-4.22347
C	-1.36734	-2.27494	-5.00354
C	1.18097	-1.60790	-5.49187
H	-1.22578	0.25777	-3.46572
H	0.42624	0.73917	-3.88294
H	-0.81297	0.65653	-5.12864
H	-1.08953	-3.32352	-5.16201
H	-2.20662	-2.27408	-4.29682
H	-1.76023	-1.90370	-5.95821
H	1.59695	-2.61786	-5.39285
H	0.87845	-1.49911	-6.54053
H	1.99565	-0.89441	-5.33109
Cl	-0.08406	-0.40617	2.40370
Na	-0.14268	-2.90881	1.83707

Calculated Structure **10**: Triplet

Mo	0.07431	-0.28969	-0.27161
P	-2.53047	-0.29727	-0.28566
P	2.68437	-0.41001	-0.24787
O	-0.06500	-1.27903	-3.22648
C	-1.33118	2.50933	0.32120
C	-0.54747	1.95684	-0.74871
C	0.85674	1.91081	-0.61171
C	1.46543	2.39580	0.59534
C	0.68881	2.91313	1.59501
C	-0.72503	2.97654	1.45421
C	-2.79548	2.49829	0.14406
C	-3.43975	1.32302	-0.27204
C	-4.82232	1.35686	-0.47846
C	-5.55686	2.51751	-0.27719
C	-4.91522	3.67254	0.16302
C	-3.54439	3.65871	0.36917
C	2.93087	2.27362	0.71571
C	3.61216	1.10923	0.30256
C	5.00721	1.08064	0.43518
C	5.71869	2.15768	0.94601
C	5.03850	3.29904	1.35734
C	3.65955	3.34875	1.24027
C	-3.55216	-1.08225	1.08378
C	-3.01725	-2.45886	1.48210
C	-3.61918	-0.17915	2.31991
C	-3.14671	-1.12379	-1.86468
C	-3.14063	-0.11599	-3.01572
C	-4.44671	-1.92600	-1.81995
C	3.64149	-1.69559	0.74333
C	3.49464	-1.47406	2.24856
C	3.29532	-3.13474	0.36601
C	3.30723	-0.74949	-1.99313
C	2.89839	0.36293	-2.96178
C	4.80098	-1.03470	-2.17303
C	0.02197	-1.11648	-2.04253
C	0.22241	-2.45201	-1.00998
H	-0.99304	1.92858	-1.73611
H	1.47079	1.88043	-1.50024
H	1.14240	3.21842	2.53124
H	-1.32852	3.34085	2.27838
H	-5.34628	0.45844	-0.78235
H	-6.62696	2.51750	-0.45203
H	-5.48099	4.58174	0.33193
H	-3.02743	4.55847	0.68511
H	5.56579	0.19785	0.15303
H	6.79851	2.10123	1.02669
H	5.58152	4.14769	1.75770
H	3.12193	4.24376	1.53280
H	-4.56325	-1.20209	0.68306
H	-2.20371	-2.32378	2.20264
H	-2.68005	-3.05534	0.63038
H	-3.79000	-3.03713	1.99549
H	-2.61694	0.08071	2.66760
H	-4.13039	-0.70973	3.12942
H	-4.16921	0.74147	2.12376
H	-2.35131	-1.83876	-2.07943
H	-3.91826	0.64126	-2.89573
H	-3.31611	-0.63178	-3.96457
H	-2.17667	0.39048	-3.09591
H	-4.45191	-2.67145	-1.02154
H	-4.55497	-2.46817	-2.76467
H	-5.33530	-1.30167	-1.70878
H	4.69421	-1.55399	0.49568
H	4.18547	-2.13031	2.78630
H	2.48079	-1.67942	2.59188
H	3.71652	-0.44455	2.53544
H	2.25847	-3.38723	0.60747
H	3.93641	-3.82555	0.92063
H	3.42854	-3.34100	-0.69950
H	2.74513	-1.64899	-2.27821
H	1.81736	0.47550	-3.02991
H	3.26431	0.12261	-3.96398
H	3.34744	1.31783	-2.67124
H	5.38771	-0.12142	-2.05612
H	4.97218	-1.39460	-3.19161
H	5.19637	-1.79390	-1.49654
H	1.24456	-2.74750	-1.27541
Si	-0.72526	-4.04378	-1.24651
H	-0.11417	-4.98918	-2.20765
H	-0.63971	-4.73472	0.09628
H	-2.17633	-3.94596	-1.51863
B	-0.45613	-2.67731	-5.28541
C	-0.62879	-1.39084	-6.18273
C	-1.76490	-3.40338	-4.77604
C	0.95799	-3.34937	-5.10675
H	-1.13942	-0.61094	-5.60794
H	0.30697	-0.96981	-6.55763
H	-1.27527	-1.59897	-7.04352
H	-1.59569	-4.19203	-4.03997
H	-2.51199	-2.70803	-4.37957
H	-2.24123	-3.88522	-5.64145
H	1.03812	-3.98279	-4.21862
H	1.14416	-3.99775	-5.97512
H	1.76801	-2.61482	-5.09155
Cl	0.03317	-0.45809	2.43582
Na	-0.05587	-2.80080	1.49952

Calculated Structure **11**: Triplet

Mo	0.04951	-0.56609	-0.36057
P	-2.66746	-0.40661	-0.36604
P	2.72998	-0.50378	-0.21650
O	0.26824	-2.17225	-3.06672
C	-1.31994	2.46222	0.09901
C	-0.62510	2.02465	-1.04050
C	0.76249	1.99199	-1.04651
C	1.48449	2.40994	0.08345
C	0.79495	2.88652	1.19007
C	-0.60079	2.90876	1.19948
C	-2.79878	2.42628	0.07542
C	-3.48969	1.25660	-0.27270
C	-4.88588	1.30839	-0.36031
C	-5.58685	2.47522	-0.09685
C	-4.89641	3.62260	0.28391
C	-3.51364	3.59384	0.36601
C	2.96146	2.33159	0.04171
C	3.62067	1.12690	-0.25077
C	5.01670	1.14416	-0.34447
C	5.74599	2.30825	-0.14880
C	5.08664	3.48949	0.17440
C	3.70375	3.49546	0.26657
C	-3.63244	-1.17303	1.06303
C	-3.09460	-2.54437	1.47995
C	-3.68819	-0.26206	2.29550
C	-3.39695	-1.16685	-1.93429
C	-3.83523	-0.12977	-2.97950
C	-4.50657	-2.20106	-1.73845
C	3.61815	-1.18158	1.29205
C	3.53917	-0.22922	2.48837
C	3.11919	-2.57025	1.68725
C	3.43686	-1.48401	-1.65127
C	3.39360	-0.61894	-2.91093
C	4.79011	-2.18179	-1.49715
C	0.20867	-1.75756	-1.88276
C	0.29263	-2.76894	-0.64581
H	-1.16731	1.77315	-1.94497
H	1.29219	1.71004	-1.95038
H	1.34622	3.18688	2.07449
H	-1.12954	3.22181	2.09305
H	-5.44143	0.41158	-0.61227
H	-6.66788	2.48688	-0.17523
H	-5.43432	4.53797	0.50198
H	-2.96392	4.49072	0.63114
H	5.55407	0.22790	-0.54946
H	6.82639	2.28896	-0.23393
H	5.64658	4.40229	0.34187
H	3.17525	4.41590	0.49092
H	-4.64888	-1.30529	0.68317
H	-2.31142	-2.39236	2.22884
H	-2.71617	-3.13963	0.64803
H	-3.88119	-3.12599	1.96744
H	-2.68367	0.01041	2.62451
H	-4.17243	-0.80442	3.11368
H	-4.25825	0.64928	2.11881
H	-2.52650	-1.68543	-2.34047
H	-4.86605	0.19014	-2.81596
H	-3.77177	-0.58114	-3.97265
H	-3.21560	0.76660	-2.99283
H	-4.24772	-2.98418	-1.02445
H	-4.70119	-2.68872	-2.69789
H	-5.44434	-1.74068	-1.41471
H	4.66628	-1.26459	0.98755
H	4.03084	-0.69163	3.34963
H	2.50236	-0.02688	2.76116
H	4.04160	0.71851	2.28934
H	2.14575	-2.47034	2.17414
H	3.79891	-3.01510	2.41884
H	3.03599	-3.25904	0.84388
H	2.69008	-2.27017	-1.79123
H	2.39451	-0.21035	-3.07919
H	3.63385	-1.22849	-3.78393
H	4.10974	0.20511	-2.85706
H	5.63261	-1.48868	-1.50274
H	4.93069	-2.84720	-2.35324
H	4.85758	-2.79690	-0.59794
H	1.32450	-3.12461	-0.52576
Si	-0.77483	-4.23469	-0.98482
H	-0.15433	-5.24374	-1.87314
H	-1.06052	-4.96786	0.30578
H	-2.10620	-3.85911	-1.51704
B	-0.12983	-1.41284	-4.45152
C	-0.48133	0.12714	-4.10263
C	-1.40132	-2.27714	-4.97615
C	1.13440	-1.58751	-5.44833
H	-1.24802	0.20053	-3.32711
H	0.38797	0.70862	-3.76660
H	-0.87393	0.63652	-4.99053
H	-1.11157	-3.30703	-5.21761
H	-2.23214	-2.34697	-4.26229
H	-1.81077	-1.84057	-5.89569
H	1.57822	-2.58824	-5.37422
H	0.80409	-1.47205	-6.48786
H	1.93638	-0.85713	-5.29915
Cl	-0.06777	-0.44933	2.38219
Na	-0.15866	-2.93094	1.75436

Calculated Structure **12**: Triplet

Mo	0.05369	-0.55947	-0.37609
P	-2.66429	-0.40118	-0.37633
P	2.73329	-0.50029	-0.22148
O	0.26188	-2.21138	-3.05288
C	-1.32010	2.46811	0.09426
C	-0.61764	2.02823	-1.04033
C	0.76986	1.99451	-1.03680
C	1.48506	2.41321	0.09776
C	0.78834	2.89025	1.19901
C	-0.60805	2.91404	1.19886
C	-2.79885	2.43206	0.06020
C	-3.48734	1.26237	-0.29386
C	-4.88309	1.31332	-0.38844
C	-5.58628	2.47947	-0.12735
C	-4.89859	3.62678	0.25851
C	-3.51621	3.59871	0.34823
C	2.96218	2.33351	0.06621
C	3.62380	1.13106	-0.23150
C	5.02080	1.14839	-0.31106
C	5.74895	2.31021	-0.09809
C	5.08702	3.48908	0.22842
C	3.70338	3.49486	0.30768
C	-3.62837	-1.15264	1.06217
C	-3.09561	-2.52249	1.49117
C	-3.68130	-0.23066	2.28655
C	-3.39817	-1.17851	-1.93388
C	-3.83887	-0.15428	-2.99102
C	-4.50664	-2.21161	-1.72486
C	3.61585	-1.19581	1.28232
C	3.52872	-0.26072	2.49148
C	3.12066	-2.59211	1.65399
C	3.44599	-1.46559	-1.66350
C	3.38631	-0.59301	-2.91719
C	4.80850	-2.14776	-1.52138
C	0.21676	-1.81713	-1.85259
C	0.30055	-2.76228	-0.69084
H	-1.15397	1.77867	-1.94891
H	1.30538	1.71421	-1.93789
H	1.33334	3.18990	2.08750
H	-1.14222	3.22778	2.08899
H	-5.43674	0.41626	-0.64355
H	-6.66691	2.49043	-0.21128
H	-5.43820	4.54156	0.47489
H	-2.96850	4.49547	0.61790
H	5.55982	0.23331	-0.51708
H	6.83018	2.29070	-0.17217
H	5.64569	4.40014	0.40910
H	3.17330	4.41364	0.53495
H	-4.64552	-1.28437	0.68390
H	-2.31661	-2.36922	2.24441
H	-2.71520	-3.12426	0.66456
H	-3.88603	-3.10002	1.97737
H	-2.67609	0.04263	2.61263
H	-4.16640	-0.76454	3.10983
H	-4.24986	0.68005	2.10169
H	-2.52793	-1.70076	-2.33612
H	-4.87217	0.16101	-2.83411
H	-3.76959	-0.61576	-3.97910
H	-3.22397	0.74513	-3.01191
H	-4.24632	-2.98747	-1.00345
H	-4.70291	-2.70897	-2.67899
H	-5.44414	-1.74888	-1.40372
H	4.66572	-1.27094	0.98199
H	4.02090	-0.73231	3.34748
H	2.49048	-0.06677	2.76418
H	4.02680	0.69215	2.30645
H	2.13943	-2.50614	2.12787
H	3.79255	-3.04136	2.39008
H	3.05508	-3.27137	0.80131
H	2.70794	-2.26001	-1.80498
H	2.37875	-0.20534	-3.08389
H	3.64109	-1.19071	-3.79423
H	4.08503	0.24549	-2.85555
H	5.64218	-1.44429	-1.53897
H	4.94747	-2.81385	-2.37720
H	4.89344	-2.75969	-0.62147
H	1.32600	-3.12770	-0.53700
Si	-0.77238	-4.24759	-0.95551
H	-0.15870	-5.29422	-1.80271
H	-1.02956	-4.91763	0.37552
H	-2.11274	-3.89809	-1.48113
B	-0.13845	-1.44324	-4.41590
C	-0.49367	0.09650	-4.06305
C	-1.41118	-2.30351	-4.95161
C	1.11812	-1.60588	-5.42743
H	-1.25027	0.16642	-3.27745
H	0.37617	0.68371	-3.73819
H	-0.90058	0.60310	-4.94618
H	-1.11674	-3.32788	-5.21092
H	-2.23930	-2.39088	-4.23633
H	-1.82626	-1.85443	-5.86261
H	1.56932	-2.60392	-5.35975
H	0.77753	-1.49023	-6.46363
H	1.91712	-0.87095	-5.28458
Cl	-0.06938	-0.43851	2.37071
Na	-0.17615	-2.91054	1.72751

Calculated Structure **13**: Triplet

Mo	0.15842	-0.32805	-0.64473
P	-2.61419	-0.31660	-0.61538
P	2.82638	-0.30008	-0.72720
O	-0.72710	-2.84392	-1.86496
C	-1.31812	2.53036	0.14034
C	-0.57584	2.08631	-0.98923
C	0.82283	2.10147	-0.96269
C	1.49791	2.51641	0.21830
C	0.76282	2.98553	1.28305
C	-0.64435	3.00347	1.24141
C	-2.79440	2.45989	0.11432
C	-3.47819	1.29762	-0.28287
C	-4.87856	1.33622	-0.32801
C	-5.59275	2.46821	0.03300
C	-4.91008	3.60212	0.46292
C	-3.52616	3.59329	0.49446
C	2.96795	2.39997	0.31675
C	3.66348	1.22982	-0.05136
C	5.05388	1.21708	0.13458
C	5.74344	2.30609	0.64780
C	5.04871	3.45565	1.00230
C	3.67509	3.49190	0.83737
C	-3.62304	-1.38177	0.56995
C	-3.30811	-2.89283	0.44643
C	-3.53832	-0.84379	2.00612
C	-3.27327	-0.82336	-2.29874
C	-3.41363	0.38200	-3.23349
C	-4.54931	-1.66439	-2.35253
C	3.78348	-1.63814	0.15844
C	3.40350	-1.67103	1.63827
C	3.61820	-3.00318	-0.51133
C	3.52735	-0.37956	-2.47624
C	3.19048	0.86942	-3.29709
C	5.03795	-0.61705	-2.58409
C	-0.04056	-2.46467	-0.77820
C	0.25845	-3.49579	0.12035
H	-1.09026	1.96885	-1.93603
H	1.38189	2.02728	-1.88443
H	1.26987	3.26890	2.19858
H	-1.20034	3.31558	2.11877
H	-5.43321	0.46167	-0.64550
H	-6.67546	2.46392	-0.01807
H	-5.45470	4.49272	0.75459
H	-2.98332	4.48353	0.79269
H	5.62996	0.33802	-0.11720
H	6.81918	2.25211	0.76951
H	5.57309	4.31695	1.39990
H	3.12232	4.38828	1.09583
H	-4.65854	-1.24715	0.25547
H	-2.52966	-3.13294	-0.28245
H	-4.19797	-3.44567	0.14573
H	-3.03926	-3.34113	1.41189
H	-2.51510	-0.65183	2.34710
H	-4.02158	-1.53886	2.69895
H	-4.04853	0.11653	2.09369
H	-2.47049	-1.46326	-2.65930
H	-4.32182	0.94800	-3.01362
H	-3.47206	0.02995	-4.26663
H	-2.57762	1.08070	-3.17604
H	-4.45234	-2.60712	-1.81719
H	-4.74277	-1.91697	-3.39878
H	-5.43263	-1.13592	-1.98585
H	4.83865	-1.36912	0.09936
H	4.01825	-2.41106	2.15822
H	2.35652	-1.93770	1.77453
H	3.55475	-0.70197	2.12000
H	2.57799	-3.32004	-0.53544
H	4.18588	-3.74890	0.05344
H	3.99036	-3.01469	-1.53713
H	3.00640	-1.23683	-2.91475
H	2.12279	0.99979	-3.46440
H	3.65699	0.78645	-4.28219
H	3.58980	1.77090	-2.82205
H	5.59468	0.29264	-2.34995
H	5.27443	-0.88000	-3.61853
H	5.41084	-1.42491	-1.95520
H	0.93374	-3.27327	0.94627
Si	-0.13695	-5.23786	-0.35739
H	0.30813	-6.13571	0.74713
H	-1.59897	-5.47156	-0.51017
H	0.52411	-5.70401	-1.59781
B	-0.20556	-2.43454	-3.27846
C	0.02758	-0.79996	-3.30770
C	-1.30677	-2.90820	-4.37440
C	1.20644	-3.20468	-3.52821
H	0.85087	-0.45315	-2.63546
H	0.43427	-0.48933	-4.27694
H	-0.86008	-0.17628	-3.15896
H	-1.62301	-3.93831	-4.17100
H	-2.21993	-2.30357	-4.45230
H	-0.86253	-2.91216	-5.37698
H	1.05255	-4.27916	-3.67769
H	1.72574	-2.83425	-4.42267
H	1.89983	-3.10982	-2.68405
Cl	0.18721	-0.16607	1.87563
Na	-1.04796	-2.36971	1.79245

Calculated Structure **14**: Triplet

Mo	0.16718	-0.32744	-0.63120
P	-2.61831	-0.31302	-0.63747
P	2.82988	-0.31675	-0.69408
O	-0.75469	-2.83193	-1.83719
C	-1.31239	2.52915	0.11061
C	-0.56256	2.06311	-1.00753
C	0.83747	2.07628	-0.97131
C	1.50349	2.50858	0.21069
C	0.76206	2.99251	1.26305
C	-0.64630	3.01441	1.20992
C	-2.78884	2.46788	0.07289
C	-3.47708	1.30608	-0.31783
C	-4.87682	1.35239	-0.37425
C	-5.58699	2.49248	-0.03110
C	-4.90056	3.62703	0.39160
C	-3.51697	3.61002	0.43460
C	2.97236	2.39176	0.32066
C	3.66830	1.21720	-0.03111
C	5.05772	1.20440	0.15987
C	5.74669	2.29821	0.66384
C	5.05161	3.45218	1.00397
C	3.67854	3.48839	0.83290
C	-3.64642	-1.37304	0.53704
C	-3.32935	-2.88458	0.42010
C	-3.57899	-0.83171	1.97327
C	-3.26247	-0.81608	-2.32824
C	-3.38965	0.38892	-3.26520
C	-4.54217	-1.65079	-2.39314
C	3.77851	-1.64676	0.21353
C	3.38209	-1.66604	1.68937
C	3.62546	-3.02012	-0.44232
C	3.54162	-0.41818	-2.43805
C	3.21714	0.82373	-3.27488
C	5.05214	-0.66287	-2.53417
C	-0.03714	-2.48663	-0.73690
C	0.25471	-3.45164	0.08382
H	-1.06937	1.94597	-1.95826
H	1.40215	2.00394	-1.88960
H	1.26232	3.28617	2.17923
H	-1.20795	3.34120	2.07847
H	-5.43445	0.47806	-0.68742
H	-6.66931	2.49441	-0.09106
H	-5.44199	4.52436	0.66852
H	-2.97102	4.50033	0.72720
H	5.63387	0.32221	-0.08082
H	6.82205	2.24485	0.78978
H	5.57544	4.31714	1.39465
H	3.12573	4.38828	1.07921
H	-4.67806	-1.24003	0.20975
H	-2.54856	-3.12368	-0.30731
H	-4.21626	-3.43961	0.11478
H	-3.06729	-3.33165	1.38867
H	-2.56094	-0.62999	2.32542
H	-4.06344	-1.52832	2.66380
H	-4.09691	0.12504	2.05335
H	-2.45905	-1.45961	-2.67958
H	-4.29505	0.96194	-3.05181
H	-3.44498	0.03505	-4.29797
H	-2.54875	1.08131	-3.20508
H	-4.45576	-2.59320	-1.85514
H	-4.72637	-1.90456	-3.44080
H	-5.42663	-1.11692	-2.03669
H	4.83393	-1.37661	0.16379
H	3.99533	-2.39658	2.22454
H	2.33505	-1.93711	1.81746
H	3.52187	-0.69101	2.16239
H	2.58770	-3.34302	-0.47149
H	4.19336	-3.75623	0.13479
H	4.00358	-3.04205	-1.46570
H	3.01960	-1.27749	-2.87130
H	2.15171	0.95857	-3.45116
H	3.69005	0.72688	-4.25575
H	3.61862	1.72805	-2.80728
H	5.61086	0.24896	-2.31349
H	5.29262	-0.94466	-3.56279
H	5.42024	-1.46043	-1.88949
H	0.89986	-3.25238	0.94150
Si	-0.16703	-5.20996	-0.36002
H	0.46542	-5.69094	-1.60676
H	0.30227	-6.08800	0.75016
H	-1.63387	-5.43378	-0.46462
B	-0.19495	-2.45732	-3.23672
C	0.05328	-0.82357	-3.28844
C	-1.27739	-2.93286	-4.35289
C	1.21783	-3.23780	-3.46262
H	0.86814	-0.46908	-2.60955
H	0.47831	-0.53066	-4.25551
H	-0.83210	-0.19159	-3.16356
H	-1.60432	-3.95957	-4.14811
H	-2.18559	-2.32367	-4.45263
H	-0.81469	-2.94672	-5.34714
H	1.06159	-4.31221	-3.61096
H	1.74824	-2.87410	-4.35341
H	1.90451	-3.14196	-2.61297
Cl	0.17358	-0.15264	1.89333
Na	-1.09831	-2.31941	1.73443

Calculated Structure **15**: Triplet

Mo	-0.02097	-0.34294	-0.41635
P	-2.67302	-0.29058	-0.25228
P	2.59324	-0.46474	-0.23730
O	-0.21768	-1.53012	-2.19305
C	-1.30073	2.57727	0.09262
C	-0.69303	1.92759	-1.02594
C	0.70880	1.86840	-1.10920
C	1.50356	2.47999	-0.08829
C	0.89449	3.12736	0.95439
C	-0.51736	3.17237	1.04733
C	-2.76992	2.54602	0.20964
C	-3.49476	1.35759	0.01691
C	-4.88995	1.41058	0.14458
C	-5.55673	2.58889	0.43873
C	-4.82945	3.76009	0.63247
C	-3.45077	3.73098	0.52113
C	2.97430	2.35225	-0.16990
C	3.58212	1.09767	-0.34088
C	4.97834	1.03140	-0.39661
C	5.76353	2.17083	-0.29687
C	5.15631	3.41022	-0.11736
C	3.77450	3.49461	-0.05380
C	-3.64705	-1.31274	1.00292
C	-3.00370	-2.68560	1.26341
C	-3.84403	-0.61389	2.35440
C	-3.33181	-0.87196	-1.91072
C	-4.64972	-0.28881	-2.41631
C	-3.39601	-2.40111	-1.96471
C	3.33504	-1.11140	1.35998
C	3.34919	-0.07067	2.48280
C	2.64170	-2.39980	1.81830
C	3.33069	-1.59738	-1.54186
C	3.64574	-0.81981	-2.82075
C	4.50563	-2.49583	-1.14755
C	0.01029	-2.36414	-1.15052
C	0.16328	-3.55362	-1.10883
H	-1.29462	1.74638	-1.91030
H	1.18013	1.62721	-2.05461
H	1.49809	3.55644	1.74714
H	-0.98123	3.62447	1.91698
H	-5.47532	0.50621	0.03091
H	-6.63757	2.59226	0.52114
H	-5.33759	4.68999	0.86112
H	-2.87367	4.64028	0.64836
H	5.46811	0.07065	-0.50313
H	6.84323	2.09140	-0.35128
H	5.75898	4.30756	-0.03513
H	3.29015	4.45734	0.06904
H	-4.62814	-1.48394	0.54733
H	-2.36352	-2.60713	2.15113
H	-2.44508	-3.08448	0.41290
H	-3.76899	-3.42206	1.51964
H	-2.88329	-0.30941	2.77481
H	-4.31446	-1.31327	3.05283
H	-4.47803	0.26762	2.29176
H	-2.53664	-0.55563	-2.58971
H	-5.50728	-0.65117	-1.84190
H	-4.79495	-0.62105	-3.44820
H	-4.66580	0.80065	-2.41107
H	-2.42677	-2.86608	-1.78253
H	-3.71586	-2.70776	-2.96161
H	-4.12653	-2.79716	-1.25297
H	4.37319	-1.34823	1.11106
H	3.72893	-0.53295	3.39931
H	2.34748	0.30819	2.68702
H	3.99822	0.77224	2.24155
H	1.78059	-2.13375	2.43903
H	3.31098	-2.99150	2.44805
H	2.33138	-3.03544	0.98081
H	2.48803	-2.25786	-1.75345
H	2.80096	-0.20988	-3.14163
H	3.86104	-1.51898	-3.63128
H	4.51067	-0.16671	-2.69354
H	5.42449	-1.93977	-0.94906
H	4.71629	-3.16785	-1.98412
H	4.29402	-3.12165	-0.27889
H	0.41215	-4.02696	-0.14583
Si	0.11664	-4.95039	-2.36249
H	1.45957	-5.25697	-2.90710
H	-0.30620	-6.14443	-1.58251
H	-0.84318	-4.76497	-3.46365
B	-0.10000	-1.53479	-3.86576
C	0.10203	0.04021	-4.17572
C	-1.47942	-2.05148	-4.54427
C	1.15202	-2.47959	-4.31452
H	-0.70418	0.65905	-3.75843
H	1.05132	0.46369	-3.83260
H	0.07306	0.20137	-5.25988
H	-1.81307	-3.04192	-4.22680
H	-2.33065	-1.36588	-4.46041
H	-1.27391	-2.13655	-5.61958
H	0.82824	-3.41702	-4.77996
H	1.75354	-1.96137	-5.07139
H	1.84852	-2.75596	-3.51907
Cl	-0.19657	-0.11894	2.15987
Na	-0.25661	-2.59800	1.38833

CRYSTALLOGRAPHIC INFORMATION

CCDC deposition numbers 1941831, 1905238, 1950973, 1950974, and 1905237 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Refinement Details

In each case, crystals were mounted on a MiTeGen loop using Paratone oil, then placed on the diffractometer under a nitrogen stream. Low temperature (100 K) X-ray data were obtained on a Bruker APEXII CCD based diffractometer (Mo-K_α radiation or Cu-K_α radiation at λ = 0.71073 Å or λ = 1.54178 Å, respectively). All diffractometer manipulations, including data collection, integration, and scaling were carried out using the Bruker APEXIII software.[21] Absorption corrections were applied using SADABS. [2222] Space groups were determined on the basis of systematic absences and intensity statistics and the structures were solved in the Olex 2 software interface[23] by intrinsic phasing using XT (incorporated into SHELXTL)[24] and refined by full-matrix least squares on F^2. All non-hydrogen atoms were refined using anisotropic displacement parameters. Hydrogen atoms were placed in the idealized positions and refined using a riding model, unless noted otherwise. The structures were refined (weighed least squares refinement on F^2) to convergence. Graphical representations of structures with 50% probability thermal ellipsoids were generated using the Diamond 3 visualization software.[25]

Table S1—Crystal and refinement data for complexes **2**, **4**, **4'**, **6** & **11**.

	2	**4**	**4'**	**6**	**11**
CCDC Number[26]	1941831	1905238	1950973	1950974	1905237
Empirical formula	$C_{45}H_{52}MoO_2P_2$	$C_{69}H_{94}Cl_2Mo_2O_2P_4$	$C_{36}H_{45}ClMoO_2P_2$	C36H42MoOP2	$C_{37}H_{55}MoOP_2Si$
Formula weight	782.74	1342.10	688.32	642.57	701.78
T (K)	100	100	100	100	100
***a*, Å**	11.665(8)	13.1011(8)	12.469(6)	23.82(2)	11.6736(5)
***b*, Å**	12.561(5)	13.0037(8)	12.592(5)	21.933(9)	12.0522(5)
***c*, Å**	13.985(6)	19.0467(12)	23.363(11)	13.402(5)	14.3227(6)
α, °	72.96(4)	90	91.78(3)°	90	94.987(2)
β, °	81.20(5)	95.462(4)	104.66(2)°	116.50(2)	105.434(2)
γ, °	88.33(4)	90	102.92(3)°	90	110.315(2)
Volume, Å^3	1935.8(18)	3230.1(3)	3444(3)	6266(7)	1785.40(13)
Z	2	2	4	8	2
Crystal system	Triclinic	Monoclinic	Triclinic	Monoclinic	Triclinic
Space group	P-1	$P2_1/n$	P-1	C12/C1	$P\bar{1}$
d_{calc}, g/cm^3	1.343	1.380	1.328	1.362	1.305
θ range, °	3.082 to 82.722	1.809 to 37.783	1.666 to 39.299	2.891 to 81.142	1.838 to 37.941
μ, mm^{-1}	0.458	0.614	0.581	4.581	0.518
Abs. Correction	Semi-empirical	Semi-empirical	Semi-empirical	Semi-empirical	Semi-empirical
GOF	1.060	1.084	1.024	1.075	1.044
R_1,[a] wR_2[b] [I>2 σ(I)]	0.0224, 0.0529	0.0339, 0.0730	0.0399, 0.0947	0.0355, 0.0966	0.0292, 0.0692
Radiation Type	Cu K_α	Mo K_α	Mo K_α	Cu K_α	Mo K_α

[a] $R_1 = \sum||F_o| - |F_c||/\sum|F_o|$. [b] $wR_2 = [\sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]]^{1/2}$

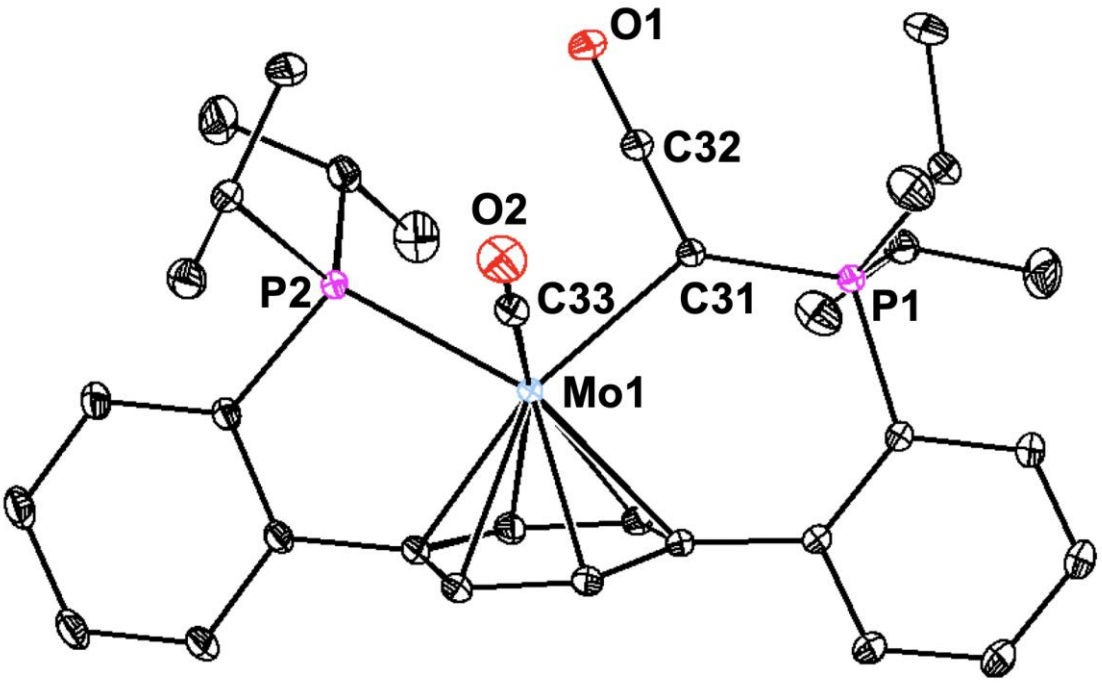


Figure S51—Structural drawing of **2** with 50% probability anisotropic displacement ellipsoids. Hydrogen atoms and benzene solvate molecules are omitted for clarity.

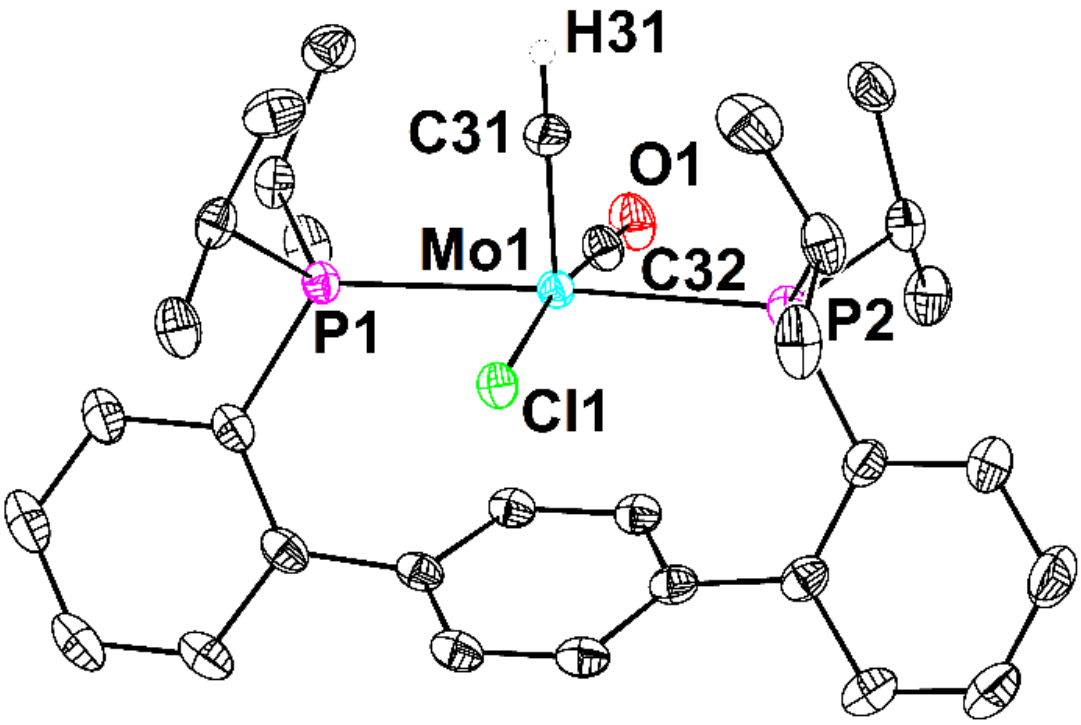


Figure S52—Structural drawing of **4** with 50% probability anisotropic displacement ellipsoids. Hydrogen atoms and a pentane solvate molecule are omitted for clarity.

Special Refinement Details for **4***:*

The methylidyne (C31), carbonyl (C32 & O1), and chloride (Cl1) ligands were positionally disordered; these disordered groups were satisfactorily modeled oved two discreet positions (A and B, Fig. S32) in a 65:35 ratio and refined without restraints.

Additionally, a disordered pentane solvate molecule was present in the crystal packing voids. Positional disorder about a symmetry special position resulted in a suitable model with four pentane molecules (each symmetry related pair sharing four carbon atoms) in a 37.5:37.5:12.5:12.5 ratio. The 1,2 distances of the minor component were restrained to be equivalent.

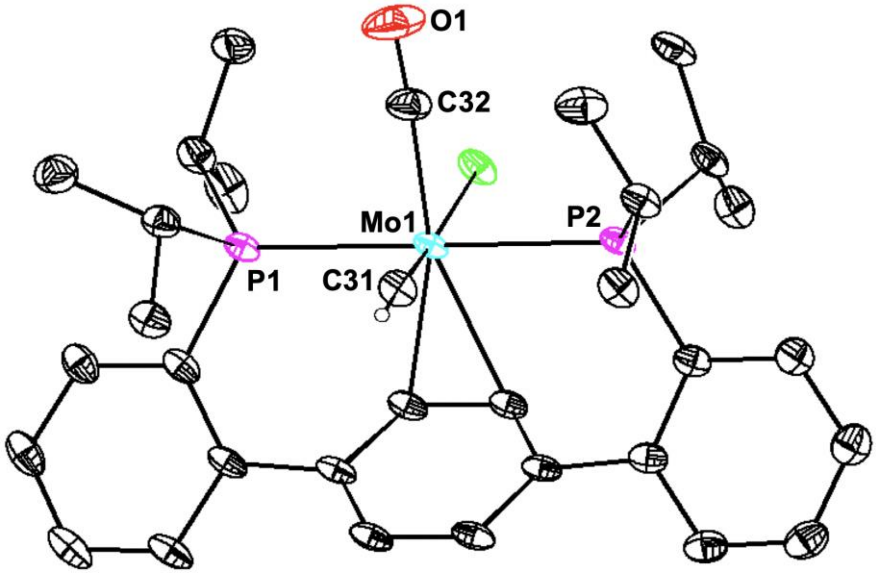


Figure S53—Structural drawing of **4'** with 50% probability anisotropic displacement ellipsoids. Hydrogen atoms and THF solvate molecules are omitted for clarity.

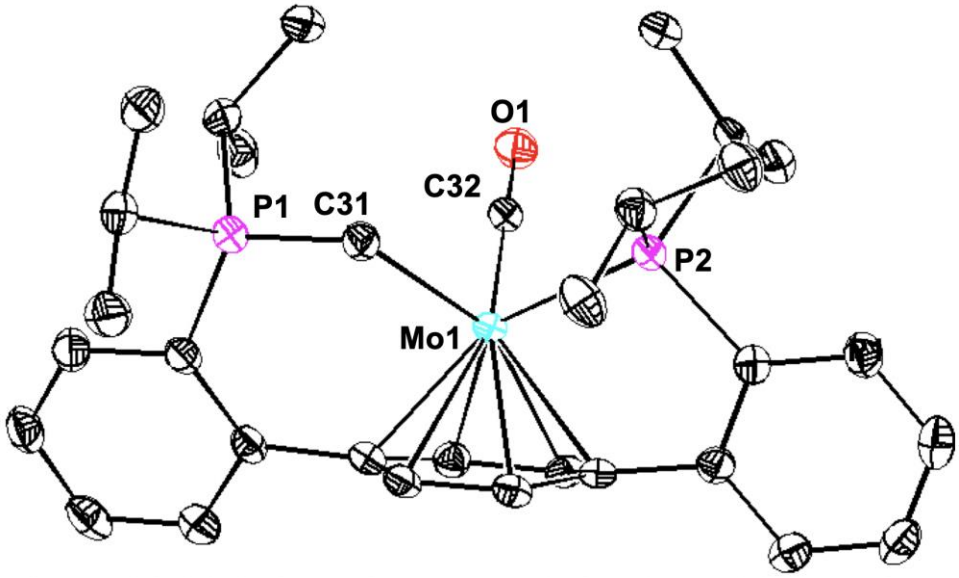


Figure S54—Structural drawing of **6** with 50% probability anisotropic displacement ellipsoids. Hydrogen atoms and toluene solvate molecules are omitted for clarity.

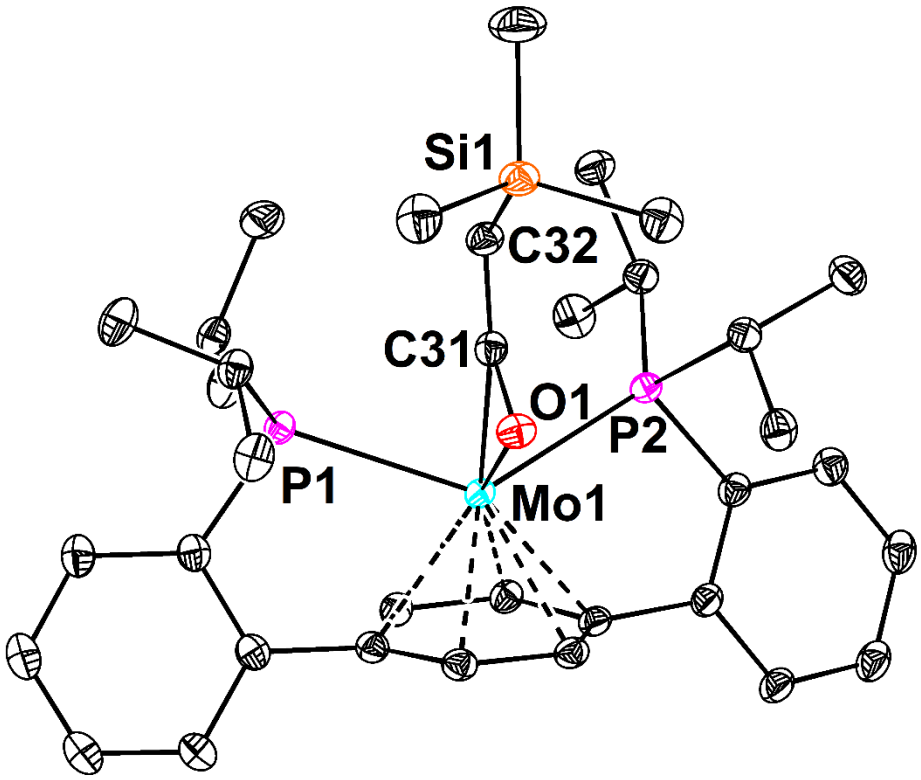


Figure S55—Structural drawing of **11** with 50% probability anisotropic displacement ellipsoids. Hydrogen atoms and a butane solvate molecule are omitted for clarity.

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